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AQUATOX MODEL DESCRIPTION

INTRODUCTION

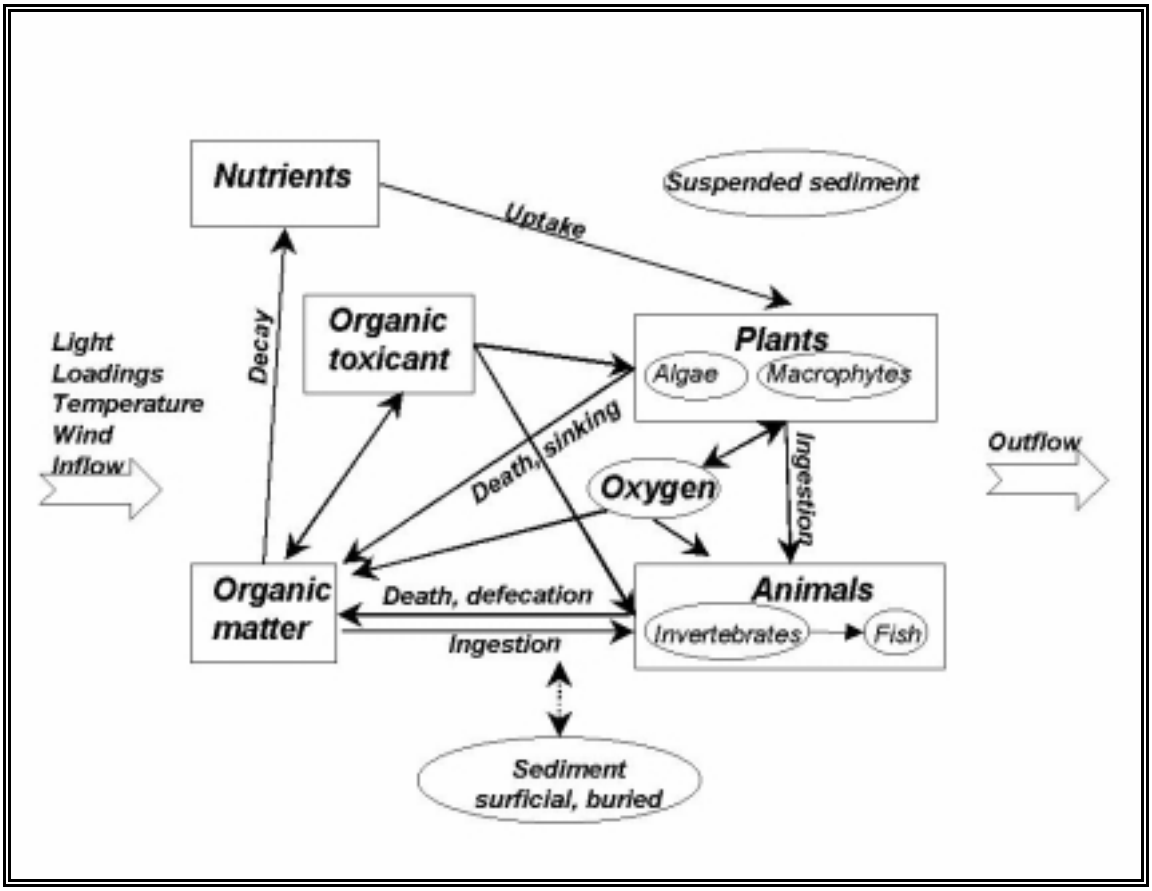
AQUATOX is a general ecological risk assessment model that represents the combined environmental fate and effects of conventional pollutants, such as nutrients, and sediments and toxic chemicals in aquatic ecosystems. This model considers several trophic levels, including attached and planktonic algae and submerged aquatic vegetation, invertebrates, and forage, bottom-feeding, and piscivorous (game) fish. This model also represents associated organic toxicants (Figure 1). AQUATOX can be implemented as a simple model (indeed, it has been used to simulate an abiotic flask) or as a truly complex food-web model. Often it is desirable to model a food web rather than a food chain, for example, to examine the possibility of less tolerant organisms being replaced by more tolerant organisms as environmental perturbations occur. "Food web models provide a means for validation because they mechanistically describe the bioaccumulation process and ascribe causality to observed relationships between biota and sediment or water" (Connolly and Glaser, 1998).

AQUATOX has been implemented for streams, small rivers, ponds, lakes, and reservoirs. This model is intended to be used to evaluate the bioaccumulation of organic contaminants and the effects of various stressors including potentially toxic organic chemicals, nutrients, organic wastes, sediments, and temperature. The stressors may be considered individually or together.

The fate portion of this model, which is applicable especially to organic toxicants, includes: partitioning among organisms, suspended and sedimented detritus, suspended and sedimented inorganic sediments, and water; volatilization; hydrolysis; photolysis; ionization; and microbial degradation. The effects portion of the model includes chronic and acute toxicity to the various organisms modeled and indirect effects such as release of grazing and predation pressure, increase in detritus and recycling of nutrients from killed organisms, dissolved oxygen sag due to increased decomposition, and loss of food base for animals.

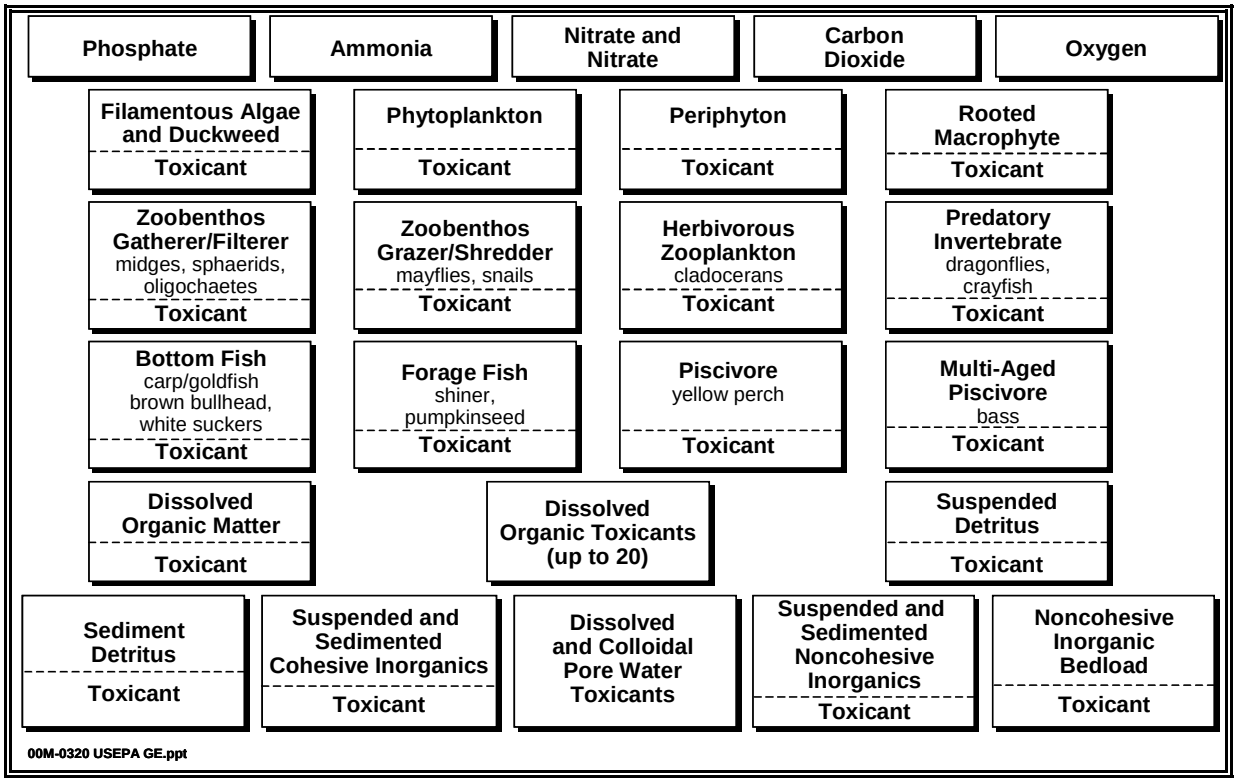
AQUATOX represents the aquatic ecosystem by simulating the changing concentrations (in mg/L or g/m^3) of organisms, nutrients, chemicals, and sediments in a unit volume of water (**Figure 1**). As such, AQUATOX differs from population models, which represent the changes in numbers of individuals. As O'Neill et al. (1986) stated, ecosystem models and population models are complementary; one cannot take the place of the other. Population models excel at modeling individual species at risk and modeling fishing pressure and other age/size-specific aspects; but recycling of nutrients, the combined fate and effects of toxic chemicals, and other interdependencies in the aquatic ecosystem are important aspects that AQUATOX represents and that cannot be addressed by a population model.

Figure 1. Conceptual Model of Ecosystem Represented by AQUATOX



Any ecosystem model consists of multiple components requiring input data. These are the abiotic and biotic **state variables** or compartments being simulated (**Figure 2**). In AQUATOX, the biotic state variables may represent trophic levels, guilds, and/or species. This model can represent a food web with both detrital- and algal-based trophic linkages. Closely related are **driving variables**, such as temperature, light, and nutrient loadings, which force the system to behave in certain ways. In AQUATOX, state variables and driving variables are treated similarly in the code. This provides flexibility because external loadings of state variables, such as phytoplankton carried into a reach from upstream, may function as driving variables; and driving variables, such as pH and temperature, could be treated as dynamic state variables in a future implementation. Constant, dynamic, and multiplicative loadings can be specified for atmospheric, point and nonpoint sources. Loadings of pollutants can be turned off to obtain a **control** simulation for comparison with the **perturbed** simulation.

Figure 2 Compartments (State Variables) in AQUATOX



AQUATOX is written in object-oriented Pascal using the Delphi programming system for Windows™. An object is a unit of computer code that can be duplicated, and the object's parameters and procedures can be inherited by higher-level objects. For example, the plant object, including variables such as the *PMax* (maximum photosynthesis rate) and process functions such as photosynthesis, is inherited by the algal object; that is, enhanced by plant-specific variables and functions and duplicated for several kinds of algae. It can also be inherited and modified slightly for macrophytes. This modularity forms the basis for the flexibility of the model, including the ability to add and delete given state variables interactively.

AQUATOX uses **differential equations** to represent changing values of state variables, normally with a reporting time step of one day. These equations require starting values or **initial conditions** for the beginning of the simulation. If the first day of a simulation is changed, then the initial conditions may need to be changed. A simulation can begin with any date and may be for any length of time from a few days, corresponding to a microcosm experiment, to decades.

The **process equations** contain another class of input variables: the **parameters** or coefficients that allow the user to specify key process characteristics. For example, the maximum consumption rate is a critical parameter characterizing various consumers. AQUATOX is a mechanistic model with many parameters; however, default values are available so that the modeler has to be concerned only with those parameters necessary for a specific risk analysis, such as characterization of a new chemical. In the pages that follow, differential equations for the state variables will be followed by process equations and parameter definitions.

Usually the reporting time step is one day, but numerical instability is avoided by allowing the step size of the integration to vary to achieve a predetermined accuracy in the solution; this is a numerical approach, and the step size is not directly related to the temporal scale of the ecosystem simulation. AQUATOX uses a fourth- and fifth-order Runge-Kutta integration routine with adaptive step size to solve the differential equations (Press et al., 1986). The routine uses the fifth-order solution to determine the error associated with the fourth-order solution; it decreases the step size (often to 15 minutes or less) when rapid changes occur and increases the step size when there are slow changes, such as in winter. However, the step size is constrained to a maximum of one day so that short-term pollutant loadings are always detected.

BACKGROUND

AQUATOX is the latest in a series of models, starting with the aquatic ecosystem model CLEAN (Park et al., 1974) and subsequently improved in consultation with numerous researchers at various European hydrobiological laboratories, resulting in the CLEANER series (Park et al., 1975, 1979; Park, 1978; Scavia and Park, 1976; Park, Collins, et al., 1980) and LAKETRACE (Collins and Park, 1989). The MACROPHYTE model, developed for the U.S. Army Corps of Engineers (Collins et al., 1985), provided additional capability for representing submersed aquatic vegetation. Another series started with the toxic fate model PEST, developed to complement CLEANER (Park, Connolly, et al., 1980, 1982), and continued with the TOXTRACE model (Park, 1984) and the spreadsheet equilibrium fugacity PART model.

AQUATOX combined algorithms from these models with ecotoxicological constructs, and additional code was written as required for a truly integrative fate and effects model (Park, 1990, 1993). AQUATOX was then restructured and linked to Microsoft Windows™ interfaces to provide greater flexibility, capacity for additional compartments, and user friendliness. AQUATOX has also been improved with the addition of constructs for chronic effects and uncertainty analysis, making this model a powerful tool for probabilistic risk assessment. AQUATOX has been validated, documented, and released by the U.S. Environmental Protection Agency (2000a, 2000b, 2000c).

Recently, AQUATOX was enhanced by doubling the number of biotic state variables so that each guild or taxonomic group could be represented by tolerant and intolerant species. Elimination of organic chemicals by organisms was also split into depuration and biotransformation. For the Housatonic River project, AQUATOX was expanded to simulate 20 chemicals simultaneously, with transformations from one to another, and to model as many as 15 age classes of one game fish and two size classes for all other fish species. AQUATOX was also made spatially explicit to model linked river tributaries, reaches, and backwater areas.

SPATIAL REPRESENTATION

AQUATOX can link several segments into one larger system. Segments can be joined in two ways. The first is a unidirectional linkage, referred to as a “cascade” link. In this case, water flows in only one direction, and there is no feedback from the lower segment to the upper segment. Segments that are linked together in this manner are solved separately from one another. The upstream segment outflow is treated as a loading into the downstream segment, along with any dissolved or particulate matter within that outflow.

The second way in which two segments can be linked is called a "feedback" link. In this case, water can flow in both directions over a segment boundary or there can be a circular link between segments. Diffusion of dissolved and suspended state variables also occurs between segments (see Equation **(5)**). Segments that are linked together as feedback segments are solved simultaneously as one large system of interacting state variables.

Simulations can include a mixture of cascade and feedback links. Only one group of segments can be linked with feedback links. However, cascade links can lead into and out of this feedback system. AQUATOX first solves all cascade segments upstream of the feedback system. Then, the feedback system of segments is solved. Finally, AQUATOX solves all segments that remain downstream of the feedback segments.

In the linked version of AQUATOX, stratification does not occur dynamically based on system characteristics. Instead, two segments can be characterized as epilimnion and hypolimnion by the user and they must also be linked together with a feedback link. These segments will then act as though they are stratified and linked throughout the simulation.

Bathymetric Approximations

The depth distribution of a water body is important because it determines the areas and volumes subject to mixing and light penetration. Within AQUATOX, a user is given a choice of employing general bathymetric relationships to represent the morphometry of an ecosystem. When simulating a river, a user often will not find the bathymetric equations to be relevant and so will choose not to employ them. One possible exception would be an impoundment within a riverine system.

When the user chooses to employ bathymetric equations, the shapes of ponds, lakes, and reservoirs are represented by idealized geometrical approximations, following the topological treatment of Junge (1966; see also Straškraba and Gnauck, 1985).

When a user chooses not to employ bathymetric equations, AQUATOX assumes that a segment is essentially represented by a given surface area. All the water and sediment below the given area make up the model segment. Because of this, a few simple equations are implied:

$$ZMean = \frac{Volume}{SurfaceArea} \quad \textbf{(1)}$$

where:

ZMean	=	mean depth (m);
Volume	=	volume of water (m^3); and
SurfaceArea	=	surface area of system (m^2).

Also, when bathymetry is not used, the euphotic zone is defined as follows:

$$FracLittoral = \frac{ZEuphotic}{ZMean} \quad \textbf{(2)}$$

where:

FracLittoral	=	fraction of site area that is within the euphotic zone (unitless);
ZEuphotic	=	depth of the euphotic zone, where primary production exceeds respiration, usually calculated as a function of extinction (m); and
ZMean	=	mean depth (m).

Washout and Wash-in

Transport out of the system, or washout, is an important loss term for nutrients, floating organisms, and dissolved toxicants in reservoirs and streams. Although it is considered separately for several state variables, the process is a general function of discharge:

$$Washout = \frac{Discharge}{Volume} \cdot State \qquad \textbf{(3)}$$

where:

Washout	=	loss due to being carried downstream ($g/m^3 \cdot d$), and
State	=	concentration of dissolved or floating state variable (g/m^3).

In a linked system, "wash-in" can occur, which is the transport of state variables into the current segment from an upstream segment due to moving water. When two segments are joined with a cascade link, the washout of the upper segment is saved for each day and used as a loading into the lower segment. When two segments are linked with a feedback link, wash-in is calculated as follows:

$$Washin = \sum_{inlinks} \left(Washout_{upstream} \cdot FracWashThisLink \cdot \frac{UpStreamVolume}{Volume} \right) \qquad \textbf{(4)}$$

where:

Washin	=	gain from all upstream segments ($g/m^3 \cdot d$);
inlinks	=	all upstream segments linked directly to this one;
$Washout_{upstream}$	=	washout of this variable from one upstream segment (g/m^3);
FracWashThisLink	=	fraction of total discharge from that segment that goes to this segment;
UpStreamVolume	=	volume of the upstream segment (m^3); and
Volume	=	volume of this segment (m^3).

Stratification and Mixing

Thermal stratification is handled in the simplest form consistent with the goals of forecasting the effects of nutrients and toxicants. Reservoirs and lakes are considered in the model to have two vertical zones: epilimnion and hypolimnion; the metalimnion zone that separates these is ignored. Instead, the thermocline, or plane of maximum temperature change, is taken as the separator; this is also known as the mixing depth (Hanna, 1990).

In a linked-mode run, stratification is defined as a condition of the system by defining one segment as the epilimnion and another linked segment as the hypolimnion. The dynamics of the system are then controlled by user input data for flow and diffusion over the thermocline. When a system is linked, diffusion between the epilimnion and hypolimnion is treated the same as diffusion between any two segments:

$$Diffusion = \frac{\frac{DispCoeff \cdot Area}{Length} \cdot (OtherSegConc - ThisConc)}{Volume} \quad \textbf{(5)}$$

where:

Diffusion	=	diffusion between two segments ($g/m^3 \cdot d$);
DispCoeff	=	dispersion coefficient (m^2 /d);
Area	=	area of interface between two segments (m^2);
Length	=	characteristic length of interface (m);
OtherSegConc	=	concentration of given compartment in other segment (g/m^3);
ThisConc	=	concentration of given compartment in this segment (g/m^3); and
Volume	=	volume of given segment (m^3).

BIOTA

The biota consist of two main groups, plants and animals; each is represented by a set of process-level equations. In turn, plants are differentiated into algae and macrophytes, represented by slight variations in the differential equations. Algae may be either phytoplankton or periphyton. Phytoplankton are subject to sinking and washout, whereas periphyton are subject to substrate limitation and scour by currents. These are treated as process-level differences in the equations.

Animals are subdivided into invertebrates and fish; the invertebrates may be pelagic invertebrates, benthic insects, or other benthic invertebrates. These groups are represented by different parameter values and by variations in the equations. Insects are subject to emergence, but benthic invertebrates are not. Fish can be represented by two size classes, usually young-of- the-year and adults, which are connected by promotion; and one fish species can be represented by up to 15 age classes.

Algae

The change in algal biomass—expressed as g/m^3 for phytoplankton, and as g/m^2 for periphyton—is a function of the loading (especially phytoplankton from upstream), photosynthesis, respiration, excretion or photorespiration, nonpredatory mortality, grazing or predatory mortality, and washout; as noted above, phytoplankton also are subject to sinking. If the system is stratified, turbulent diffusion also affects the biomass of phytoplankton:

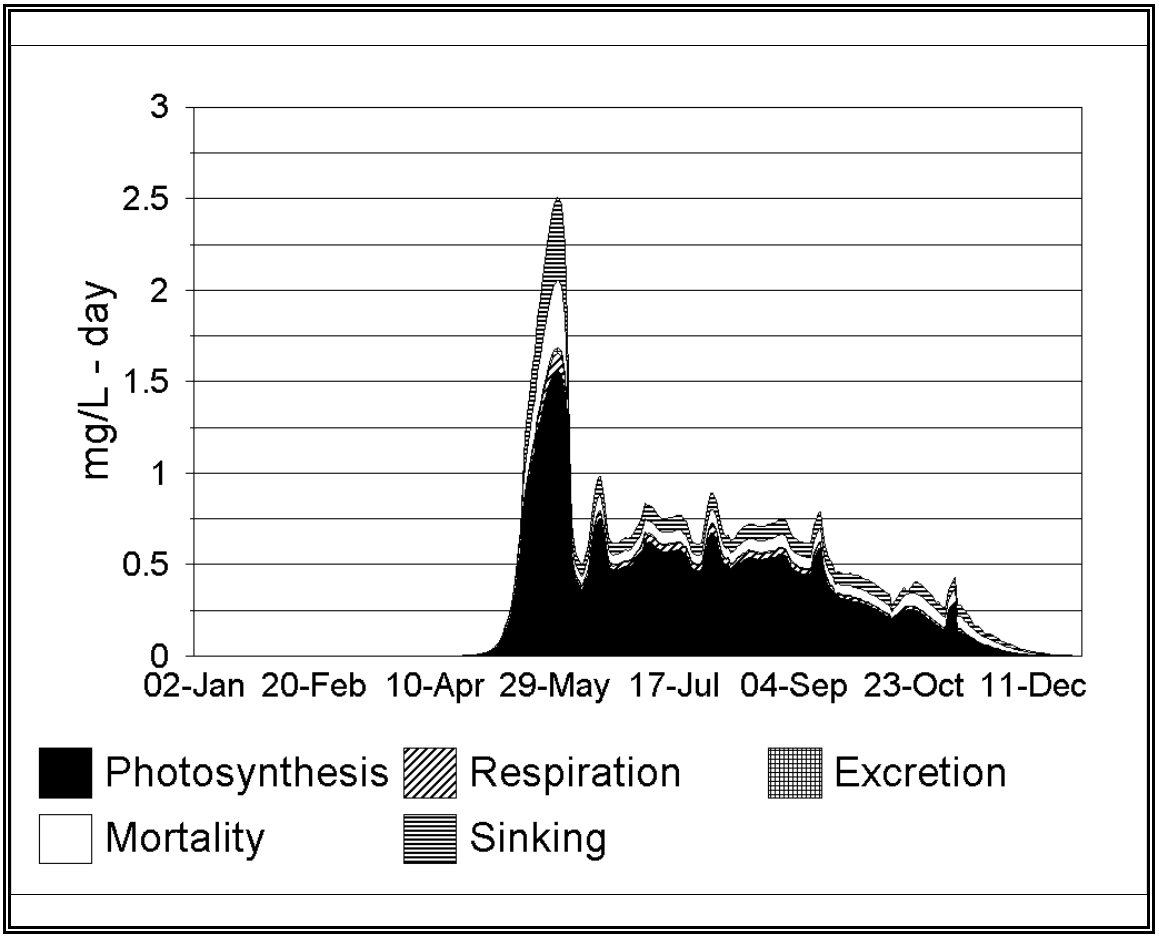
$$\frac{dBiomass}{dt} = Loading + Photosynthesis - Respiration - Excretion - Mortality - Predation \pm Sinking - Washout + Washin - Floodloss \pm TurbDiff \quad \textbf{(6)}$$

where:

dBiomass/dt	=	change in biomass of algae with respect to time ($g/m^3 \cdot d$);
Loading	=	loading of algal group ($g/m^3 \cdot d$);
Photosynthesis	=	rate of photosynthesis ($g/m^3 \cdot d$);
Respiration	=	respiratory loss ($g/m^3 \cdot d$);
Excretion	=	excretion or photorespiration ($g/m^3 \cdot d$);
Mortality	=	nonpredatory mortality ($g/m^3 \cdot d$);
Predation	=	herbivory ($g/m^3 \cdot d$);
Washout	=	loss due to being carried downstream ($g/m^3 \cdot d$);
Washin	=	addition from upstream ($g/m^3 \cdot d$);
Floodloss	=	loss overbank during flood event ($g/m^3 \cdot d$);
Sinking	=	loss or gain due to sinking between layers and sedimentation to bottom ($g/m^3 \cdot d$); and
TurbDiff	=	turbulent diffusion ($g/m^3 \cdot d$).

Figure 3 is an example of changes in the processes that contribute to changes in the predicted biomass in a eutrophic lake.

Figure 3
Predicted Algal Process Rates



Phytoplankton are subject to downstream drift. In streams, and in lakes and reservoirs with low retention times, this may be a significant factor in reducing or even precluding phytoplankton

populations (Le Cren and Lowe-McConnell, 1980). Periphyton (and macrophytes, as discussed in the next section) also may be subject to entrainment and transport as they outgrow their substrate and as discharge increases (McIntire, 1968, 1973). Because periphyton are limited by the area of substrate available, as the biomass approaches the carrying capacity of the substrate, AQUATOX predicts that increasing quantities are dislodged and available for transport.

Macrophytes

Submerged aquatic vegetation, or macrophytes, can be an important component of shallow aquatic ecosystems. It is not unusual for the majority of the biomass in an ecosystem to be in the form of macrophytes during the growing season. Seasonal macrophyte growth, death, and decomposition can affect nutrient cycling, and detritus and oxygen concentrations; macrophytes can also sequester contaminants. By forming dense cover, they can modify habitat and provide protection from predation for invertebrates and smaller fish (Howick et al., 1993); this function is represented in AQUATOX. Macrophytes also provide direct and indirect food sources for many species of waterfowl, including ducks and coots (Jupp and Spence, 1977b).

AQUATOX represents macrophytes as occupying the littoral zone, that area of the bottom surface that occurs within the euphotic zone. Similar to periphyton, the compartment has units of g/m^2. In nature, macrophytes can be greatly reduced if phytoplankton blooms or higher levels of detritus increase the turbidity of the water (Jupp and Spence, 1977a). Because the depth of the euphotic zone is computed as a function of the extinction coefficient, the area predicted to be occupied by macrophytes can increase or decrease depending on the clarity of the water. Periphyton are epiphytic in the presence of macrophytes; by growing on the leaves, they contribute to the light extinction for the macrophytes (Sand-Jensen, 1977). Extinction due to periphyton biomass is computed in AQUATOX. The macrophyte equations are based on submodels developed for the International Biological Program (Titus et al., 1972; Park et al., 1974) and CLEANER models (Park, Collins, et al., 1980) and for the Corps of Engineers CE-QUAL-R1 model (Collins et al., 1985).

Animals

Zooplankton, benthic invertebrates, benthic insects, and fish are modeled, with only slight differences in formulations, with a generalized animal submodel that is parameterized to represent different groups:

$$\frac{dBiomass}{dt} = Load + Consumption - Defecation - Respiration - Excretion - Death - Predation - GameteLoss + Washin - Washout - Floodloss \pm Migration - Promotion + Recruit \quad (7)$$

where:

dBiomass/dt	=	change in biomass of animal with respect to time ($g/m^3 \cdot d$);
Load	=	biomass loading, usually from upstream ($g/m^3 \cdot d$);
Consumption	=	consumption of food ($g/m^3 \cdot d$);
Defecation	=	defecation of unassimilated food ($g/m^3 \cdot d$);

Respiration	=	respiration ($g/m^3 \cdot d$);
Excretion	=	excretion ($g/m^3 \cdot d$);
Death	=	nonpredatory mortality ($g/m^3 \cdot d$);
Predation	=	predatory mortality ($g/m^3 \cdot d$);
GameteLoss	=	loss of gametes during spawning ($g/m^3 \cdot d$);
Washout	=	loss due to being carried downstream by washout and drift ($g/m^3 \cdot d$);
Washin	=	addition from upstream ($g/m^3 \cdot d$);
Floodloss	=	loss overbank during flood event ($g/m^3 \cdot d$);
Migration	=	loss (or gain) due to vertical migration ($g/m^3 \cdot d$);
Promotion	=	promotion to next size class or emergence ($g/m^3 \cdot d$); and
Recruit	=	recruitment from previous size class ($g/m^3 \cdot d$).

The change in biomass (**Figure 4**) is a function of a number of processes (**Figure 5**) that are subject to environmental factors, including biotic interactions. Similar to the way algae are treated, parameters for different species of invertebrates and fish are loaded and available for editing by means of the entry screens.

Figure 4
Change in Animal Biomass in Stream

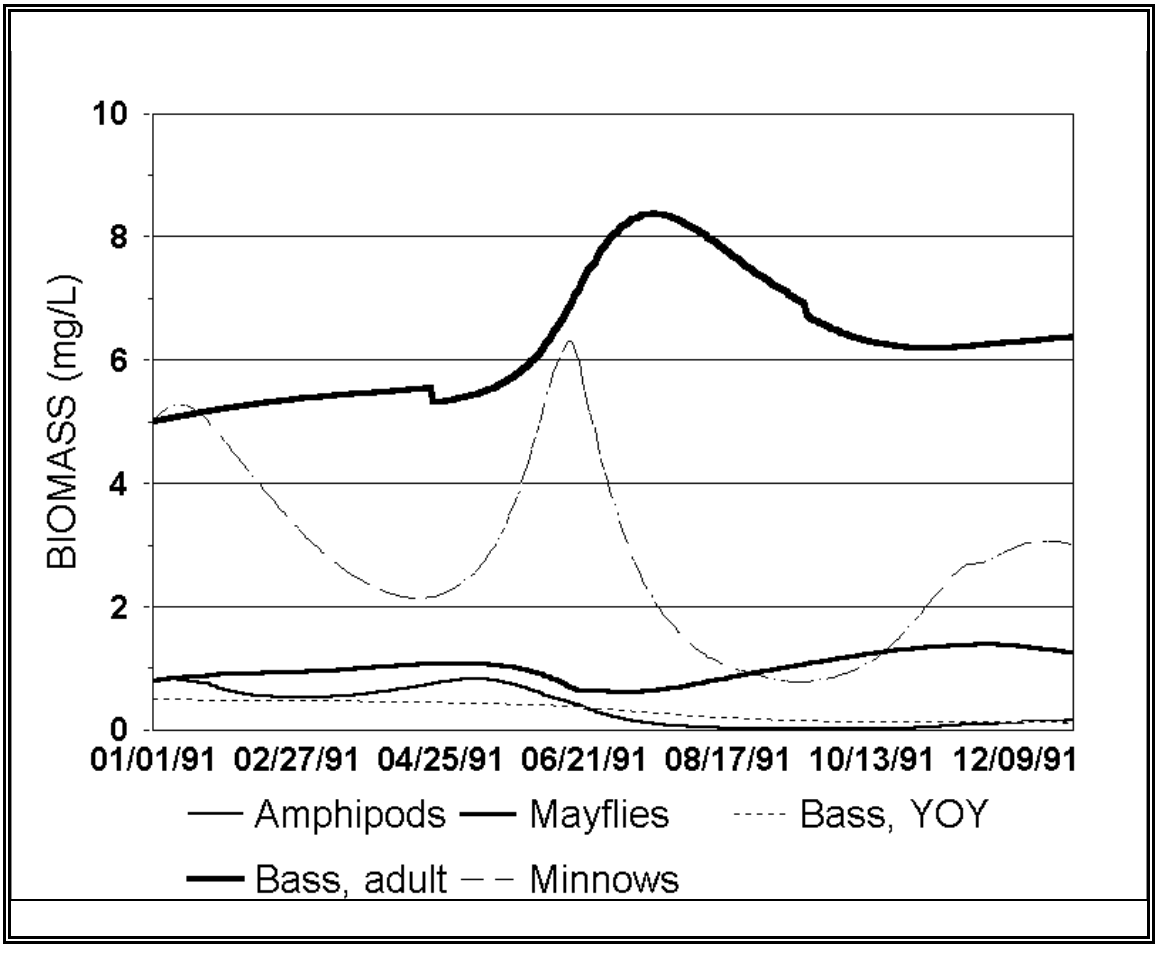
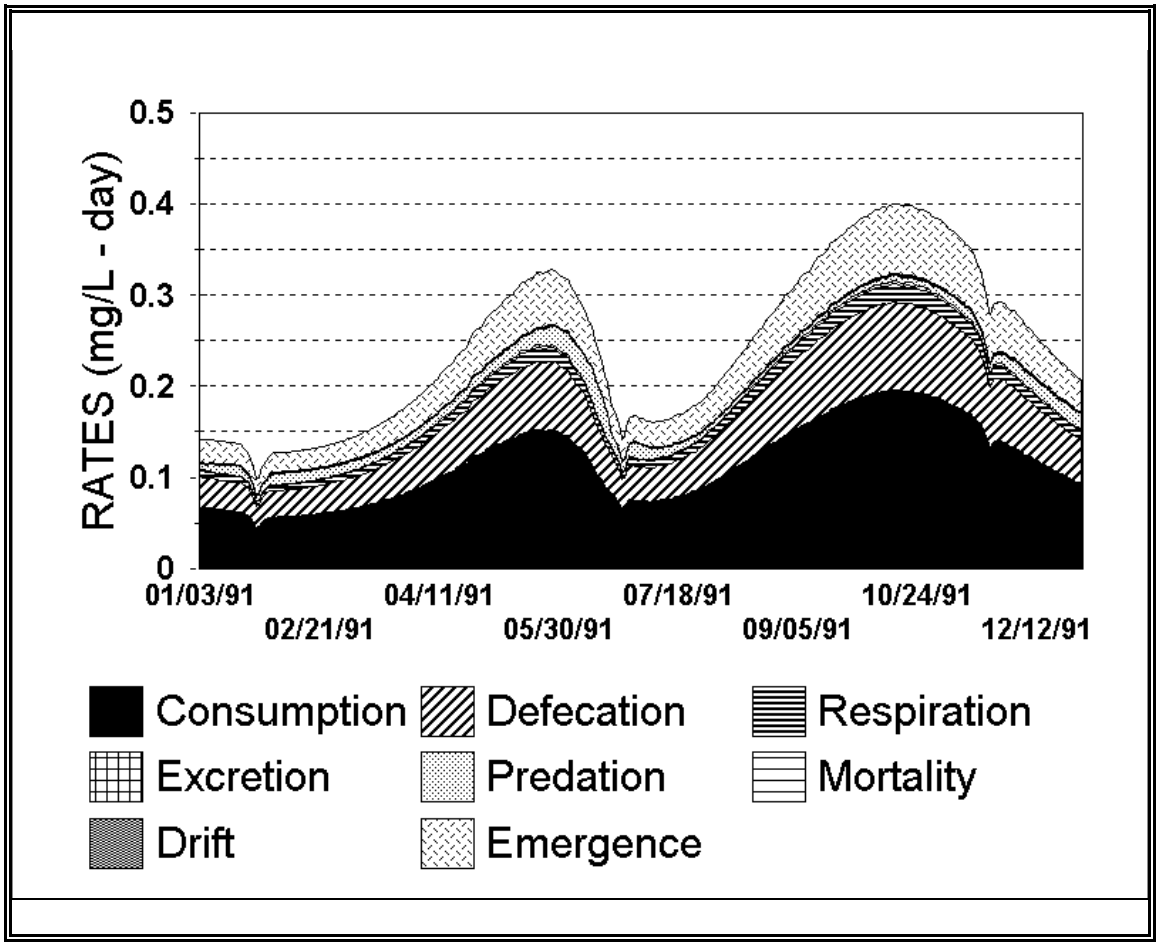


Figure 5
Mayfly Processes



Many animals adjust their search or filtration rate in accordance with the concentration of prey; therefore, a saturation-kinetic term is used (Park et al., 1974; Scavia and Park, 1976; Park, Collins, et al., 1980):

$$SatFeeding = \frac{Preference_{prey,\ pred} \cdot Food}{\Sigma_{prey}(Preference_{prey,\ pred} \cdot Food) + FHalfSat_{pred}} \quad \textbf{(8)}$$

where:

Sat Feeding	=	maximum feeding factor based on food availability (unitless);
$Preference_{prey,\ pred}$	=	preference of predator for prey (unitless);
Food	=	available food (g/m^3); and
$FhalfSat_{pred}$	=	half-saturation constant for feeding by a predator (g/m^3).

The food actually available to a predator may be reduced in two ways:

$$Food = (Biomass_{prey} - BMin_{pred}) \cdot Refuge \quad \textbf{(9)}$$

where:

$Biomass_{prey}$ = concentration of organism (g/m^3 d);
$BMin_{pred}$ = minimum prey biomass needed to begin feeding (g/m^3); and
Refuge = reduction factor for prey hiding in macrophytes (unitless).

Search or filtration may virtually cease below a minimum prey biomass (*BMin*) to conserve energy, so that a minimum food level is incorporated (Parsons et al., 1969; Steele, 1974; Park et al., 1974; Scavia and Park, 1976; Scavia et al., 1976; Steele and Mullin, 1977).

Macrophytes can provide refuge from predation (Howick et al., 1993); this is represented by a factor related to the macrophyte biomass:

$$Refuge = 1 - \frac{Biomass_{Macro}}{Biomass_{Macro} + HalfSat} \quad \textbf{(10)}$$

where:

HalfSat = half-saturation constant ($20\ g/m^3$); and
$Biomass_{Macro}$ = biomass of macrophyte (g/m^3).

AQUATOX is a food-web model with multiple potential food sources. Passive size-selective filtering and active raptorial selection occur among aquatic organisms. Relative preferences are represented in AQUATOX by a matrix of preference parameters first proposed by O'Neill (1969) and used in several aquatic models (Bloomfield et al., 1973; Park et al., 1974; Canale et al., 1976; Scavia et al., 1976). Higher values indicate increased preference by a given predator for a particular prey compared to the preferences for all possible prey. In other words, the availability of the prey is weighted by the preference factor.

The preference factors are normalized so that if a potential food source is not modeled or is below the *BMin* value, the other preference factors are modified accordingly, representing adaptive preferences:

$$Preference_{prey,pred} = \frac{Pref_{prey,pred}}{SumPref} \quad \textbf{(11)}$$

where:

$Preference_{prey,pred}$ = normalized preference of given predator for given prey (unitless);
$Pref_{prey,\ pred}$ = initial preference value from the animal parameter screen (unitless); and
SumPref = sum of preference values for all food sources that are present above the minimum biomass level for feeding during a particular time step (unitless).

Similarly, different prey types have different potentials for assimilation by different predators. The fraction of ingested prey that is egested as feces or discarded (and which is treated as a source of

detritus by the model) is indicated by a matrix of egestion coefficients with the same structure as the preference matrix.

Downstream transport is an important loss term for invertebrates. Zooplankton are subject to transport downstream similar to phytoplankton. Likewise, many zoobenthic invertebrates exhibit nocturnal drift. Both processes are represented in AQUATOX.

When presented with anoxic conditions, most animals will attempt to migrate to an adjacent area with more favorable conditions. The current version of AQUATOX, following the example of CLEANER (Park, Collins, et al., 1980), assumes that zooplankton and fish will exhibit avoidance behavior by migrating vertically from an anoxic hypolimnion to the epilimnion. The construct calculates the absolute mass of the given group of organisms in the hypolimnion, then divides by the volume of the epilimnion to obtain the biomass being added to the epilimnion.

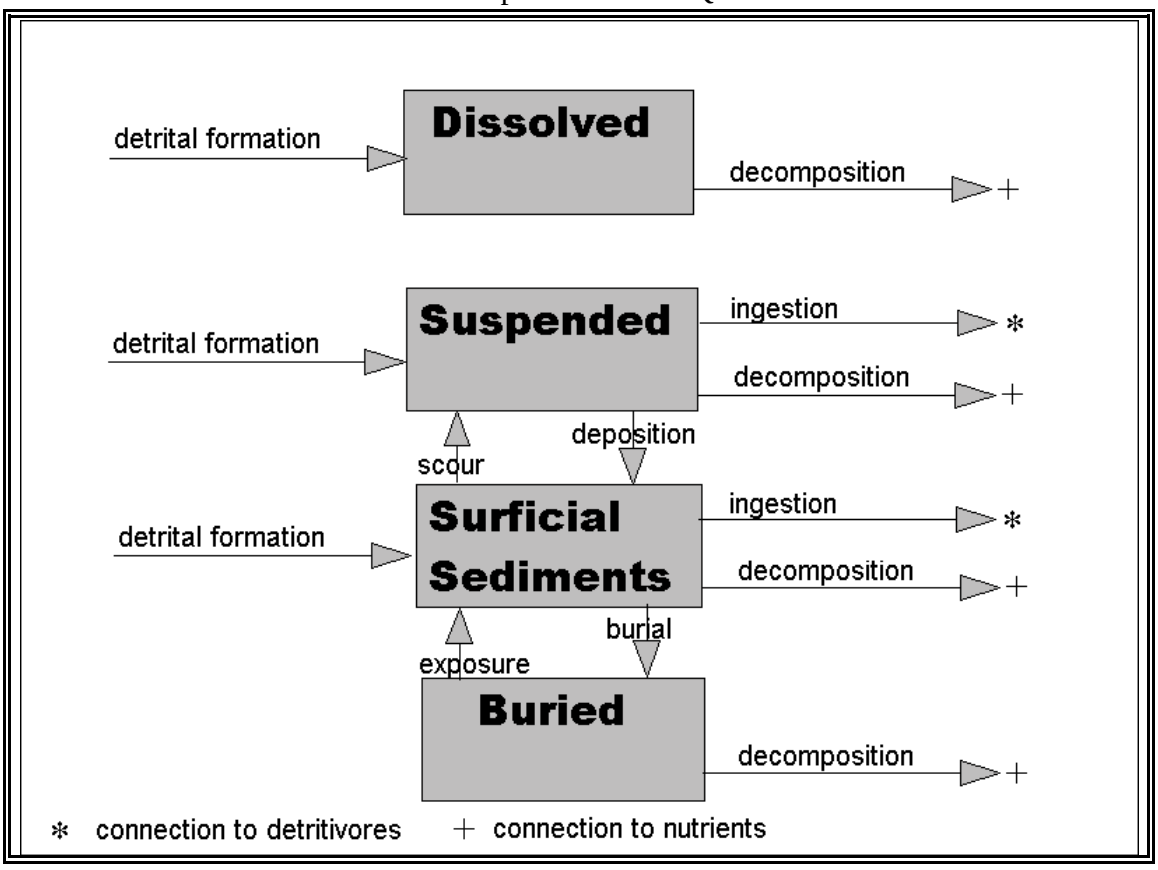
Although AQUATOX is an ecosystem model, promotion to the next size class is important in representing the emergence of aquatic insects, and therefore loss of biomass from the system, and in predicting bioaccumulation of hydrophobic organic compounds in larger fish. The model assumes that promotion is determined by the rate of growth. Growth is considered to be the sum of consumption and the loss terms other than mortality and migration; a fraction of the growth goes into promotion to the next size class (cf. Park, Collins, et al., 1980). Insect emergence can be an important factor in the dynamics of an aquatic ecosystem. Often there is synchrony in the emergence; in AQUATOX this is assumed to be cued to temperature or specified by the user.

REMINERALIZATION

Detritus

The term "detritus" is used to include all non-living organic material and associated decomposers (bacteria and fungi); as such, it includes both particulate and dissolved material in the sense of Wetzel (1975), but it also includes the microflora and is analogous to “biodetritus” of Odum and de la Cruz (1963). Detritus can be modeled as dissolved, suspended, sedimented, and buried detritus (**Figure 6**). Buried detritus is considered to be taken out of active participation in the functioning of the ecosystem. In general, the mass of dissolved organic material is about 10 times that of suspended particulate matter in lakes and streams (Saunders, 1980); however, the proportions are modeled dynamically.

Figure 6
Detrital Compartments in AQUATOX



Note: Dissolved Detritus is in Water Column and Pore Water

Decomposition is the process by which detritus is broken down by bacteria and fungi, yielding constituent nutrients, including nitrogen, phosphorus, and inorganic carbon. Therefore, it is a critical process in modeling nutrient recycling. In AQUATOX, following a concept first advanced by Park et al. (1974), the process is modeled as a first-order equation with multiplicative limitations for suboptimal environmental conditions. The model accounts for both decreased and increased degradation rates under anaerobic conditions. Detritus will always decompose more slowly under anaerobic conditions; but some organic chemicals, such as some halogenated compounds (Hill and McCarty, 1967), will degrade more rapidly.

Biomass of bacteria is not explicitly modeled in AQUATOX. In some models (for example, EXAMS, Burns et al., 1982), decomposition is represented by a second-order equation using an empirical estimate of bacteria biomass. However, using bacterial biomass as a site constant constrains the model, potentially forcing the rate. Decomposers were modeled explicitly as a part of the CLEAN model (Clesceri et al., 1977). However, if conditions are favorable, decomposers can double in 20 minutes; this can result in stiff equations, adding significantly to the computational time. Ordinarily, decomposers will grow rapidly as long as conditions are favorable. The only time the biomass of decomposers might need to be considered explicitly is when a new organic chemical

is introduced and the microbial assemblage requires time to become adapted to using it as a substrate.

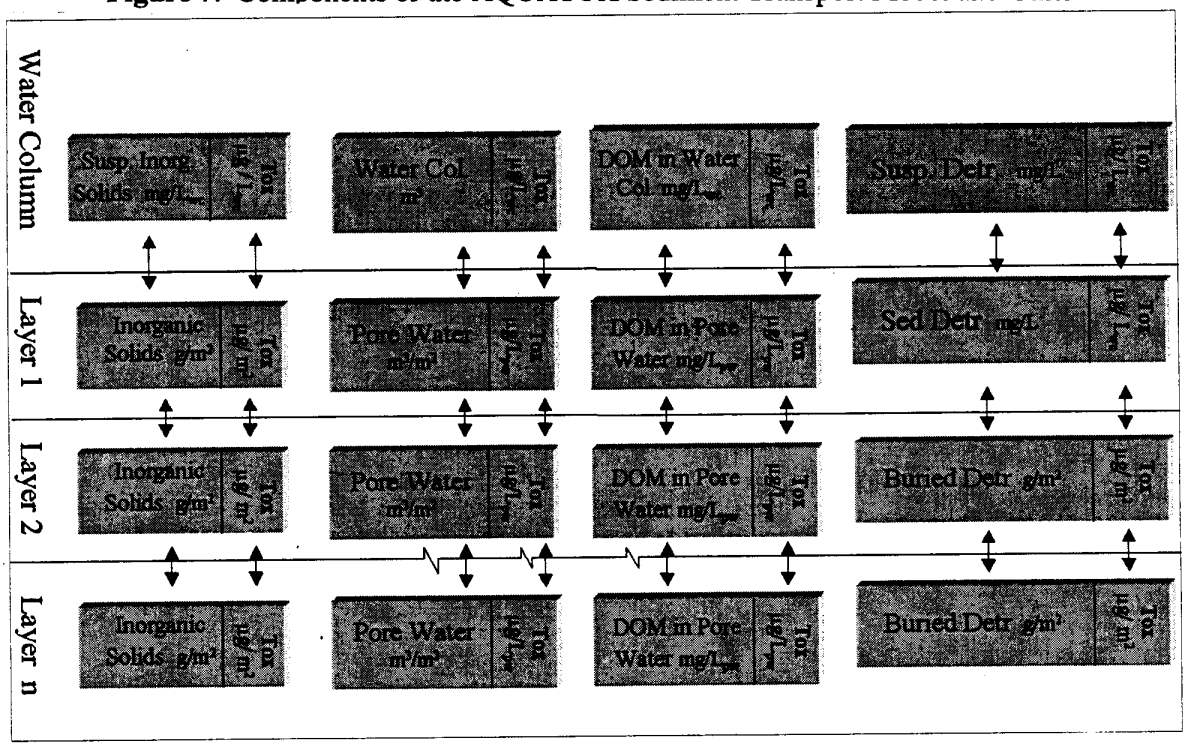
SEDIMENTS

Inorganic sediments are important to the functioning of natural and perturbed ecosystems for several reasons. When suspended, they increase light extinction and decrease photosynthesis. When sedimented, they can temporarily or permanently remove toxicants from the active ecosystem through deep burial. Rapid sedimentation can adversely affect periphyton and some zoobenthos. Scour can also adversely affect periphyton and zoobenthos.

AQUATOX models up to 10 bottom layers of sediment. Within each sediment layer, the state variables consist of inorganic solids, pore water, dissolved organic matter in pore water, and sedimented detritus. Each of these state variables can also have up to 20 organic toxicant concentrations associated with it. The AQUATOX sediment transport component is summarized in **Figure 7.**

For backwards compatibility, the AQUATOX model can be run without the sediment transport model included. In this case, the state variable that represents the active layer of sedimented detritus remains in the model, but there are no other state variables that represent the sediment of the system.

Figure 7. Components of the AQUATOX Sediment Transport Model and Units



The Sediment Transport Model

Within AQUATOX, inorganic sediments are represented as three distinct state variables as defined below:

Cohesives:	particle size smaller than 63 microns
Non-Cohesives:	particle size from 63 to 250 microns
Non-Cohesives2:	particle size greater than 250 microns

For each inorganic compartment, the sediment transport model accepts daily input parameters for interactions between the top sediment layer and the water column. These interactions are input as daily scour and daily deposition for each inorganic sediment type in units of grams per day. The model also requires deposition and erosion velocities for cohesive inorganic sediments. These inputs are then used to calculate the deposition and erosion of organic matter within the system.

AQUATOX assumes that the density of each sediment layer will remain constant throughout a simulation. Because of this, the volume and thickness of the top bed layer will vary in response to deposition and erosion.

When the top layer has reached a maximum thickness, it is broken into two layers. Other layers in the system are moved down one layer without disturbing their concentrations or thicknesses. This allows the model to maintain a contaminant-concentration gradient within the sediment layers during depositional regimes. Similarly, when the top layer has eroded to a minimum size, the layer beneath it is joined with the active layer to form a new top layer. In this case, lower layers are moved up one level, without changing their concentrations, densities, or thicknesses. More details about these processes can be found in **Sediment Interactions**, below.

At the bottom of the system, a hardpan barrier is assumed. The model, therefore, has no interaction beneath its lowest layer. If enough erosion takes place so that this hardpan barrier is exposed, no further erosion will be possible. Deposition can, however, rebuild the sediment layer system. This hardpan bottom prevents the artificial inclusion of “clean” sediment and organic matter into the simulation during erosional events. Because it is a barrier and not a boundary, it prevents loss of toxicant to the system under depositional regimes.

AQUATOX writes output data for a fixed number of sediment layers. When, due to deposition, a layer is buried below the fixed number of sediment layers, AQUATOX keeps track of that layer, but does not write daily output. When, due to erosion, there are fewer than the fixed number of sediment layers, AQUATOX writes zeros for all layers below the hardpan barrier.

Pore water moves up and down through the sediment system when layers move upward and downward in the system. Substances dissolved in pore water also move through the system as a result of diffusion.

Suspended Inorganic Sediments

As mentioned above, inorganic sediments are broken into three sets of state variables based on particle size. Each of these three inorganic sediment types is found in the water column as well as in each modeled sediment layer.

For inorganic sediments suspended in the water column, the derivative is as follows:

$$\frac{d\mathit{SuspSediment}}{dt} = \mathit{Loading} + \mathit{Scour} - \mathit{Deposition} - \mathit{Washout} + \mathit{Washin} - \mathit{Floodloss} \quad \textbf{(12)}$$

where:

d*SuspSediment*/d*t*	=	change in concentration of suspended sediment ($g/m^3 \cdot d$);
Loading	=	inflow loadings (excluding upstream segments) ($g/m^3 \cdot d$);
Scour	=	scour from the active sediment layer ($g/m^3 \cdot d$);
Deposition	=	deposition to the active sediment layer ($g/m^3 \cdot d$);
Washout	=	loss due to being carried downstream ($g/m^3 \cdot d$);
Washin	=	loadings from upstream segments ($g/m^3 \cdot d$); and
FloodLoss	=	loss to the floodplain during a flood event ($g/m^3 \cdot d$).

For each of the three categories of suspended sediment, deposition to and scour from the active layer are input to AQUATOX as a daily time series in units of g/d. These inputs are converted into units of $g/m^3 \cdot d$ by dividing by the volume of the segment.

Inorganics in the Sediment Bed

Inorganic sediments are found in each sediment layer that is modeled. The derivative for the active (top) layer is:

$$\frac{d\mathit{BottomSediment}}{dt} = \mathit{Deposition} - \mathit{Scour} + \mathit{Bedload} - \mathit{Bedloss} \quad \textbf{(13)}$$

where:

d*BottomSediment*/d*t*	=	change in concentration of sediment in this bed layer ($g/m^2 \cdot d$);
Deposition	=	deposition from the water column ($g/m^2 \cdot d$);
Scour	=	movement to the water column ($g/m^2 \cdot d$);
Bedload	=	bedload from all upstream segments ($g/m^2 \cdot d$); only relevant for the active layer of sediment; and
Bedloss	=	loss due to bedload to all downstream segments ($g/m^2 \cdot d$); only relevant for the active layer of sediment.

Deposition and scour are input into the model in units of g/d. These inputs are divided by the area of the system to get units of $g/m^2 \cdot d$.

Bedload is input as a loading in g/d for each link between two segments. This process is only relevant for the top layer of sediment modeled. The total bedload for a particular segment can be calculated by summing the loadings over all incoming links.

$$BedLoad = \sum \frac{BedLoad_{Upstreamlink}}{AvgArea} \quad \textbf{(14)}$$

where:

$BedLoad$	=	total bedload from all upstream segments ($g/m^2 \cdot d$);
$BedLoad_{Upstreamlink}$	=	bedload over one of the upstream links (g/d); and
$AvgArea$	=	average area of the segment (m^2).

Similarly, total bed loss is the sum of the loadings over all outgoing links:

$$BedLoss = \sum \frac{BedLoss_{Downstreamlink}}{AvgArea} \quad \textbf{(15)}$$

where:

$BedLoss$	=	total bedloss to all downstream segments ($g/m^2 \cdot d$);
$BedLoss_{Downstreamlink}$	=	bedload over one of the downstream links (g/d); and
$AvgArea$	=	average area of the segment (m^2).

The derivative presented is relevant only for the active layer. Inorganic sediments below the active layer do move up and down through the system as a result of exposure or deposition. However, these sediments move as a part of their entire intact layer when the active layer has reached its maximum or minimum level.

When the top layer reaches a minimum thickness, the layer below the active layer is added to the active layer to form one new layer. The inorganic sediments within these two layers do undergo mixing, represented by weighted averages of properties and constituents.

Detritus in the Sediment Bed

State variables tracking sedimented detritus are also included in each layer of sediment that is simulated. Like inorganic sediments, buried detritus below the active layer only moves up and down in the system when its layer moves up and down intact. Therefore, detritus found below the active layer has a very simple derivative:

$$\frac{dBuriedDetritus}{dt} = - Decomp \quad \textbf{(16)}$$

where:

d*BuriedDetritus*/d*t*	=	change in concentration of sediment on bottom ($g/m^2 \cdot d$); and
Decomp	=	microbial decomposition in ($g/m^2 \cdot d$).

Pore Waters in the Sediment Bed

Pore waters are also tracked in the sediment beds. Pore waters below the top layer only move when the enclosing layer moves up or down. The derivative for pore waters in the top layer is:

$$\frac{d PoreWater}{dt} = Gain_{Up} - Loss_{Up} \quad \textbf{(17)}$$

where:

d*PoreWater*/d*t*	=	change in volume of pore water in the sediment bed normalized per unit area ($m^3/m^2 \cdot d$);
$Gain_{Up}$	=	gain of pore water from the water column above ($m^3/m^2 \cdot d$); and
$Loss_{Up}$	=	loss of pore water to the water column above ($m^3/m^2 \cdot d$).

In the active layer, pore waters are assumed to move into the water column when scour occurs. To keep the density constant, the same fraction of pore water must be released as the fraction of sediment that has been scoured:

$$Loss_{Up} = \frac{\sum SedScour}{\sum SedMass} \cdot PoreWater \quad \textbf{(18)}$$

where:

$Loss_{Up}$	=	loss of pore water to the water column above ($m^3/m^2 \cdot d$);
SedScour	=	scour of all sediment to the water column above, (g/d);
SedMass	=	mass of all sediment in the active layer, (g); and
PoreWater	=	volume of pore water in the sediment bed normalized to unit area (m^3/m^2).

Pore waters are also squeezed into the water column when the active layer reaches a maximum thickness and is split into two layers. The bottom of these two new layers is assumed to be compressed and pore water is released as a result. More details about this process can be found in **Sediment Interactions** below.

Pore waters are taken from the water column when deposition occurs. This process is also required to maintain the constant density of the top sediment layer. To keep the density constant, the same fraction of pore water must be deposited as the fraction of sediment that has been deposited:

$$Gain_{Up} = \frac{\sum SedDeposition}{\sum SedMass} \cdot PoreWater \quad \textbf{(19)}$$

where:

$Gain_{Up}$	=	gain of pore water from the water column above ($m^3/m^2 \cdot d$);
SedDeposition	=	deposition of all sediment to the water column above, (g/d);
SedMass	=	mass of all sediment in the active layer, (g); and
PoreWater	=	volume of pore water in the sediment bed normalized to unit area (m^3/m^2).

Dissolved Organic Matter within Pore Waters

Another state variable tracked within the sediment bed is dissolved organic matter within pore waters of the respective layers. Like other dissolved detritus compartments, these variables use units of mg/L. However, it is important to note that these are liters of pore water and not liters in the water column.

$$\frac{d\,DOM_{PoreWater}}{dt} = GainDOM_{Up} - LossDOM_{Up} + Diff_{Down} - Diff_{Up} - Decomp \qquad \textbf{(20)}$$

where:

$dDOM_{PoreWater}/dt$	=	change in concentration of DOM in pore water in the sediment bed normalized per unit area ($mg/L_{pw} \cdot d$);
$GainDOM_{Up}$	=	active layer only: gain of DOM due to pore water gain from the water column ($mg/L_{pw} \cdot d$);
$LossDOM_{Up}$	=	active layer only: loss of DOM due to pore water loss to the water column ($mg/L_{pw} \cdot d$);
$Diff_{Down}$	=	diffusion over the lower boundary ($mg/L_{pw} \cdot d$);
$Diff_{Up}$	=	diffusion over upper boundary ($mg/L_{pw} \cdot d$); and
Decomp	=	microbial decomposition ($mg/L_{pw} \cdot d$).

The increase of DOM due to pore water gain from the water column is simply the volume of water that is moving from the water column above multiplied by the DOM concentration in the water column. However, the concentration then needs to be normalized for the volume of pore water in the current segment:

$$GainDOM_{up} = (Conc_{DOM\ n-1})\ (GainPW_{up})\ \frac{AvgArea \cdot 1E3}{PoreWaterVol} \qquad \textbf{(21)}$$

where:

$GainDOM_{Up}$	=	gain of DOM due to pore water gain from the layer above ($mg/L_{pw} \cdot d$);
$Conc_{DOM-1}$	=	concentration of DOM in above layer ($mg/L_{upper\ water}$);
$GainPW_{up}$	=	gain of pore water from above ($m^3_{upper\ water}/m^2 \cdot d$);
AvgArea	=	average area of the segment (m^2);
1 E 3	=	units conversion (L/m^3); and
PoreWaterVol	=	pore water volume (L).

The loss of DOM in pore water to the water column is a simpler equation because no unit conversions are necessary:

$$LossDOM_{up} = Conc_{DOM\,n} \frac{LossPW_{up}}{PoreWaterConc} \quad \textbf{(22)}$$

where:

$LossDOM_{Up}$	=	loss of DOM due to pore water movement to the layer above ($mg/L_{pw}\cdot d$);
$Conc_{DOM\,n}$	=	concentration of DOM in this layer (mg/L_{pw});
$LossPW_{up}$	=	loss of pore water to above layer ($m^3_{pw}/m^2\cdot d$); and
$PoreWaterConc$	=	pore water concentration (m^3_{pw}/m^2).

Because diffusion and decomposition of DOM in pore water occur throughout the system, this derivative is relevant for the whole system. DOM in pore water also moves up and down through a system when its layer moves intact due to erosion or deposition.

Sediment Interactions

The mass of the top sediment layer increases and decreases as a result of deposition and scour. Therefore, the volume and thickness of the top sediment layer also increases and decreases. When the thickness of the top sediment layer reaches its maximum, as defined by the user, the upper bed is split into two layers. The top of these two layers maintains the same density it had before the layer was split up. It is assigned the initial condition depth of the active layer.

The lower level is assumed to be compressed to the same density as the level below it. This compression results in pore water being squeezed into the water column. The volume that is lost as a result of this compression can be solved as follows:

$$VolumeLost = Volume_{new2} - Volume_{new2} \cdot \frac{Density_{active}}{Density_{lower}} \quad \textbf{(23)}$$

where:

$VolumeLost$	=	volume of active layer lost due to compaction (m^3);
$Volume_{new2}$	=	volume of the new second layer before compression (m^3);
$Density_{active}$	=	density of the active layer (g/m^3); and
$Density_{lower}$	=	density of the lower below the active layer (g/m^3).

This equation also provides the quantity of pore water squeezed into the water column because the compression of the active layer is entirely the result of pore water being squeezed out. If there is only one layer in the system when the splitting of the active layer takes place, $Density_{lower}$ is assumed to be the initial condition density of the second layer in the system.

The volume of a sediment layer is defined as follows:

$$BedVol_n = \frac{\sum SedMass}{BedDensity} \quad \textbf{(24)}$$

where:

$BedVol_n$	=	volume of bed at layer n (m^3);
SedMass	=	mass of sediment type (g); and
BedDensity	=	density of bed (g/m^3).

The porosity of a sediment layer is defined as:

$$FracWater_n = 1 - \sum_{Sedtypes} (Conc_{sed} / Density_{sed}) \quad \textbf{(25)}$$

where:

$FracWater_n$	=	porosity of the sediment layer (fraction);
Sedtypes	=	all organic and inorganic sediments;
$Conc_{sed}$	=	concentration of the sediment (g/m^3); and
$Density_{sed}$	=	density of the sediment (g/m^3).

When the thickness of the top sediment layer reaches a minimum, as defined by the user, the two top layers combine into one new active layer. The density of this new layer is the weighted average of the two existing layers. This allows the layers to be combined while requiring no additional pore-water interactions.

The bottom of the system is a hardpan barrier. When this bottom is exposed, no further erosion can take place. When deposition occurs on this hardpan bottom, it is rebuilt with the density of the layer that existed previously. If enough deposition occurs so that two layers are created, the new second layer is compressed to the density of the original second layer.

If a system starts with exposed hardpan as an initial condition, the user must still specify the density of the top layer to be used when the top layer is created. If the user specifies a density for the second layer, this will be used when enough deposition occurs so that two layers are created.

TOXIC ORGANIC CHEMICALS

The chemical fate module of AQUATOX predicts the partitioning of a compound between water, sediment, and biota, and estimates the rate of degradation of the compound. Photolysis, hydrolysis, microbial degradation, and volatilization are modeled in AQUATOX. The latter two processes are especially applicable to PCBs and are discussed in greater detail below.

Microbial degradation is modeled by entering a maximum biodegradation rate for a particular organic toxicant, which is subsequently reduced to account for suboptimal temperature, pH, and dissolved oxygen. Photolysis is modeled by using a light-screening factor (Schwarzenbach et al.,

1993) and the near-surface, direct photolysis first-order rate constant for each pollutant. The light screening factor is a function of both the diffuse attenuation coefficient near the surface and the average diffuse attenuation coefficient for the whole water column. For those organic chemicals that undergo hydrolysis, neutral, acid-, and base-catalyzed reaction rates are entered into AQUATOX as applicable. Volatilization is modeled using a stagnant two-film model, with the air and water transfer velocities approximated by empirical equations based on reaeration of oxygen (Schwarzenbach et al., 1993).

The mass balance equations are presented below. The change in mass of toxicant in the water includes explicit representations of degradation pathways, mobilization of the toxicant from sediment to water as a result of decomposition of the sediment detritus compartment, sorption to and desorption from the detrital sediment compartments, uptake by algae and macrophytes, uptake across the gills of animals, depuration by organisms, advective transport and diffusion between segments, transfer to and from pore water, net loss to the floodplain, and turbulent diffusion between epilimnion and hypolimnion:

$$\begin{aligned}\frac{dToxicant_{Water}}{dt} = {} & Loading + \sum_{Detr}(Decomposition_{Detr} \cdot PPB_{Detr} \cdot 1E-6) \\ & + \sum Desorption_{DetrTox} + \sum_{Org}(K2 \cdot PPB_{Org} \cdot 1E-6) \\ & - \sum Sorption_{DetrTox} - \sum GillUptake_{Pred} - MacroUptake \\ & - \sum AlgalUptake_{Alga} - Hydrolysis - Photolysis - MicrobialDegrdn \\ & - Volatilization - Discharge + TurbDiff + Inflow \\ & + MicrobTrans \pm Diffusion - Floodloss \pm PoreWaterTransfer\end{aligned} \quad (26)$$

The equations for the toxicant associated with sedimented detritus compartments are rather involved:

$$\begin{aligned}\frac{dToxicant_{SedDetritus}}{dt} = {} & Sorption - Desorption \\ & + \sum_{Pred}\sum_{Prey}\left(Def2Detr \cdot DefecationTox_{Pred,\ Prey}\right) \\ & - (Resuspension + Decomposition) \cdot PPB_{SedDetritus} \cdot 1E-6 \\ & - \sum_{Pred} Ingestion_{Pred,\ SedDetritus}) \cdot PPB_{SedDetritus} \cdot 1E-6 \\ & + Sedimentation \cdot PPB_{SuspDetritus} \cdot 1E-6 \\ & + \sum(Sed2Detr \cdot Sink_{Phyto} \cdot PPB_{Phyto} \cdot 1E-6) \\ & - Hydrolysis - MicrobialDegrdn \\ & \mp MicrobTrans - Burial + Expose\end{aligned} \quad (27)$$

Similarly, for the toxicant associated with suspended particulate and dissolved detritus, the equations are:

$$\frac{d\,Toxicant_{DissolvedDetr}}{dt} = Loading + Sorption - Desorption + \sum ExcrToxToDiss_{Org} + \sum_{Org} (Mort2Detr \cdot Mortality_{Org} \cdot PPB_{Org} \cdot 1E-6) - (Washout + Decomposition) \cdot PPB_{DissolvedDetr} \cdot 1E-6 + Inflow + MicrobTrans \pm Diffusion \pm PoreWaterTransfer - FloodLoss - Hydrolysis - Photolysis - MicrobialDegrdn + TurbDiff \quad (28)$$

$$\frac{d\,Toxicant_{SuspDetr}}{dt} = Loading + Sorption - Desorption + \sum_{Pred} (Def2Sed \cdot Def_{Pred}) + \sum_{Org} ((Mort2Detr \cdot Mortality_{Org} + GameteLoss_{Org}) \cdot PPB_{Org} \cdot 1E-6) - (Sedimentation + Washout + Decomp + \sum_{Pred} Ingestion_{Pred,\ SuspendedDetr}) \cdot PPB_{SuspendedDetr} \cdot 1E-6 + Resuspension \cdot PPB_{SedimentedDetr} \cdot 1E-6 - SedToHyp + SedFrEpi + MicrobTrans + Inflow \pm Diffusion - FloodLoss - Hydrolysis - Photolysis - MicrobialDegrdn + TurbDiff \quad (29)$$

Algae are represented as:

$$\frac{d\,Toxicant_{Alga}}{dt} = Loading + AlgalUptake - Depuration + TurbDiff + (- Excretion - Washout - \sum_{Pred} Predation_{Pred,\ Alga} - Mortality - Sink + SinkToHypo - SinkFrEpi) \cdot PPB_{Alga} \cdot 1E-6 \pm Diffusion \pm Biotransformation + Inflow - Floodloss \quad (30)$$

Macrophytes are represented similarly, but they move only if they are floating macrophytes. Otherwise, they are stationary:

$$\frac{d\,Toxicant_{Macrophyte}}{dt} = Loading + MacroUptake - Depuration - (Excretion + \sum_{Pred} Predation_{Pred,\ Macro} + Mortality + Washout) \cdot PPB_{Macro} \cdot 1E-6 \pm Biotransformation + Inflow - Floodloss \quad (31)$$

The toxicant associated with animals is represented by a kinetic equation because of the various routes of exposure and transfer:

$$\frac{dTox_{Animal}}{dt} = Loading + GillUptake + \sum_{Prey} DietUptake + TurbDiff - (Depuration + \sum_{Pred} Predation_{Pred,\ Animal} + Mortality + Spawn \pm Promotion + Drift + Migration + EmergeInsect) \cdot PPB_{Animal} \cdot 1E-6 \pm Diffusion - Floodloss \quad (32)$$

where:

PPB_{Alga}	=	concentration of toxicant in given alga (μg/kg);
$Toxicant_{SedDetr}$	=	mass of toxicant associated with the sediment detritus compartments in unit volume of water (μg/L);
$Toxicant_{SuspDetr}$	=	mass of toxicant associated with the suspended detritus compartments in unit volume of water (μg/L);
$Toxicant_{DissDetr}$	=	mass of toxicant associated with the dissolved organic compartments in unit volume of water (μg/L);
$Toxicant_{Alga}$	=	mass of toxicant associated with given alga in unit volume of water (μg/L);
$Toxicant_{Macrophyte}$	=	mass of toxicant associated with given macrophyte in unit volume of water(μg/L);
$Toxicant_{Animal}$	=	mass of toxicant associated with given animal in unit volume of water (μg/L);
$PPB_{SedDetr}$	=	concentration of toxicant in sediment detritus (μg/kg);
$PPB_{SuspDetr}$	=	concentration of toxicant in suspended detritus (μg/kg);
$PPB_{DissDetr}$	=	concentration of toxicant in dissolved organics (μg/kg);
$Toxicant_{Water}$	=	toxicant in dissolved phase in unit volume of water (μg/L);
$PPB_{Macrophyte}$	=	concentration of toxicant in given macrophyte (μg/kg);
PPB_{Animal}	=	concentration of toxicant in given animal (μg/kg);
1 E -6	=	units conversion (kg/mg);
Loading	=	loading of toxicant from external sources (μg/L·d);
TurbDiff	=	depth-averaged turbulent diffusion between epilimnion and hypolimnion (μg/L·d);
Inflow	=	flow of toxicant from upstream linked segments (μg/L·d);
MicrobTrans	=	microbial transformation of another toxicant type to this toxicant type (μg/L·d);
Diffusion	=	diffusion over segment boundaries. If the toxicant is in a dissolved phase and if the sediment bed model is included, this term includes diffusion to or from the active layer (μg/L·d);
Biotransformation	=	biotransformation to or from this toxicant within an organism (μg/L·d);
Floodloss	=	loss to the floodplain during a flood event (μg/L·d);
PoreWaterTransfer	=	transfer to or from pore water in the active layer during deposition or erosion (μg/L·d);
Hydrolysis	=	rate of loss due to hydrolysis (μg/L·d);
Photolysis	=	rate of loss due to direct photolysis (μg/L·d);

MicrobialDegrdn	=	rate of loss due to microbial degradation (μg/L·d);
Volatilization	=	rate of loss due to volatilization (μg/L·d);
Discharge	=	rate of loss of toxicant due to discharge downstream (μg/L·d);
Burial	=	rate of loss due to deep burial (μg/L·d);
Expose	=	rate of exposure due to resuspension of overlying sediments (μg/L·d);
Decomposition	=	rate of decomposition of given detritus (mg/L·d);
Depuration	=	elimination rate for toxicant due to clearance (μg/L·d);
Sorption	=	rate of sorption to given compartment (μg/L·d);
Desorption	=	rate of desorption from given compartment (μg/L·d);
$DefecationTox_{Pred, Prey}$	=	rate of transfer of toxicant due to defecation of given prey by given predator (μg/L·d);
Def2Detr	=	fraction of defecation that goes to given compartment;
Resuspension	=	rate of resuspension of given sediment detritus (mg/L·d);
Sedimentation	=	rate of sedimentation of given suspended detritus (mg/L·d);
Sed2Detr	=	fraction of sinking phytoplankton that goes to given detrital compartment;
Sink	=	loss rate of phytoplankton to bottom sediments (mg/L·d);
Death	=	nonpredatory mortality of given organism (mg/L·d);
Mort2Detr	=	fraction of dead organism that is labile (unitless);
GameteLoss	=	loss rate for gametes (g/m^3·d);
Washout or *Drift*	=	rate of loss of given suspended detritus or organism due to being carried downstream (mg/L·d);
SedToHyp	=	rate of settling loss to hypolimnion from epilimnion (mg/L·d);
SedFrEpi	=	rate of gain to hypolimnion from settling out of epilimnion (mg/L·d);
$Ingestion_{Pred, Prey}$	=	rate of ingestion of given food or prey by given predator (mg/L·d);
$Predation_{Pred, Prey}$	=	predatory mortality by given predator on given prey (mg/L·d);
$ExcToxToDiss_{Org}$	=	toxicant excretion from plants to dissolved organics (mg/L·d);
Excretion	=	excretion rate for given organism (g/m^3·d);
SinkToHypo	=	rate of transfer of phytoplankton to hypolimnion (mg/L·d);
SinkFrEpi	=	loss rate of phytoplankton to hypolimnion (mg/L·d);
AlgalUptake	=	rate of sorption by algae (μg/L·d);
MacroUptake	=	rate of sorption by macrophytes (μg/L·d);
GillUptake	=	rate of absorption of toxicant by the gills (μg/L·d);
$DietUptake_{Prey}$	=	rate of dietary absorption of toxicant associated with given prey (μg/L·d);
Promotion	=	promotion from one age class to the next (mg/L·d);
Migration	=	rate of migration (g/m^3·d); and
EmergeInsect	=	insect emergence (mg/L·d).

The derivatives for toxicants in the sediment transport component of AQUATOX are described below.

$$\frac{\mathrm{d}Toxicant_{Porewater}}{\mathrm{d}t} = GainTox_{up} - LossTox_{up} \pm DiffUp \pm DiffDown + \sum_{Detr\ n}(Decomposition_{Detr\ n} \cdot PPB_{Detr\ n} \cdot 1E-6) + \sum Desorption_{DetrTox\ n} + \sum_{Org\ n}(K2 \cdot PPB_{Org\ n} \cdot 1E-6) - \sum Sorption_{DetrTox\ n} - \sum GillUptake_{Pred\ n} - MicrobialDegrdn + MicrobTransfIn \quad (33)$$

$$\frac{\mathrm{d}Toxicant_{SuspSediment}}{\mathrm{d}t} = Scour/Volume \cdot PPB_{ActiveLayer} \cdot 1E-6 - Deposition/Volume \cdot PPB_{SuspSediment} \cdot 1E-6 - (Washout - Floodloss) \cdot PPB_{SuspSediment} \cdot 1E-6 + WashinTox - MicrobialDegrdn + MicrobTransfIn \quad (34)$$

$$\frac{\mathrm{d}Toxicant_{BottomSediment}}{\mathrm{d}t} = Deposition/AvgArea \cdot PPB_{UpperLayer} \cdot 1E-3 - Scour/AvgArea \cdot PPB_{ThisLayer} \cdot 1E-3 + ToxBedLoad - ToxBedLoss - MicrobialDegrdn + MicrobTransfIn \quad (35)$$

$$\frac{\mathrm{d}Toxicant_{BuriedDetritus}}{\mathrm{d}t} = -Decomposition \cdot PPB_{ThisLayer} \cdot 1E-3 - MicrobialDegrdn + MicrobTransfIn + Sorption - Desorption \quad (36)$$

$$\frac{dToxicant_{DOM\ Porewater}}{dt} = GainTox_{up} - LossTox_{up} \pm DiffUp \cdot PPB_{DOM\ init\ layer} \cdot 1E-6 \pm DiffDown \cdot PPB_{DOM\ init\ layer} \cdot 1E-6 + Sorption - Desorption - MicrobialDegrdn + MicrobTransfIn - Decomposition \cdot PPB_{DissLabileDetr\ pore\ water} \cdot 1E-6\ (if\ labile) \quad (37)$$

where:

$Toxicant_{SuspSediment}$	=	toxicant within suspended sediments (μg/L);
Scour/Volume	=	scour from the active sediment layer normalized to unit volume ($g/m^3 \cdot d$);
Deposition/Volume	=	deposition to the active sediment layer normalized to unit volume ($g/m^3 \cdot d$);
$PPB_{SuspSediment}$	=	concentration of toxicant in suspended sediment (μg/kg);
$PPB_{ActiveLayer}$	=	concentration of toxicant in this state variable in the top layer of sediment (μg/kg);
1 E -6	=	units conversion (kg/mg);
Washout	=	loss due to being carried downstream ($g/m^3 \cdot d$);
FloodLoss	=	loss to the floodplain during a flood event ($g/m^3 \cdot d$);
WashinTox	=	toxicant loadings from upstream segments ($g/m^3 \cdot d$);
MicrobialDegrdn	=	rate of loss due to microbial degradation (μg/L·d);
MicrobTransfIn	=	rate of gain due to microbial transformation of another chemical to this chemical type (μg/L·d);
Scour/AvgArea	=	scour from this sediment layer normalized to unit area ($g/m^2 \cdot d$);
Deposition/AvgArea	=	deposition to this sediment layer normalized to unit area ($g/m^2 \cdot d$);
$PPB_{ThisLayer}$	=	concentration of toxicant in this state variable in this layer of sediment (μg/kg);
$PPB_{UpperLayer}$	=	concentration of toxicant in this state variable in the layer above this layer of sediment (μg/kg);
$PPB_{init\ layer}$	=	concentration of toxicant in the given state variable in the layer where diffusive movement originates (μg/kg);
1 E -3	=	units conversion (kg/g);
Exposure	=	movement up from lower sediment layer ($g/m^2 \cdot d$);
Burial	=	movement down to lower sediment layer ($g/m^2 \cdot d$);
ToxBedLoad	=	toxicant bedload from upstream segments (μg/L·d);
ToxBedLoss	=	toxicant bedloss to downstream segments (μg/L·d) ;
$Deposition_{Detr}$	=	deposition of detritus to this layer from the above layer (g/m^2);
$Scour_{Detr}$	=	scour of detritus from this layer to the above layer (g/m^2);
Decomposition	=	rate of decomposition of given detritus, relevant to labile detritus only (mg/L·d);
Sorption	=	rate of sorption to given compartment (μg/L·d);
Desorption	=	rate of desorption from given compartment (μg/L·d);
$GainTox_{up}$	=	gain of toxicant from above layer due to pore water transport (μg/L·d); and
$LossTox_{up}$	=	loss of toxicant to below layer due to pore water transport (μg/L·d).

The wash-in of toxicants in carriers from upstream segments is calculated by summing the total toxins in carriers that wash over each of the upstream segment links.

$$WashinTox_{Thisvar} = \sum Washout_{Upstreamlink} \cdot PPB_{Upstreamvar} \cdot 1E-6 \quad \textbf{(38)}$$

where:

$WashinTox_{Thisvar}$	=	total toxicant in this state variable that is washed into this segment from all upstream links (µg/L·d);
$Washout_{Upstreamlink}$	=	washout of this state variable from this particular upstream segment (g/m^3·d);
$PPB_{Upstreamvar}$	=	toxicant in this state variable in the upstream segment (µg/kg); and
1 E -6	=	units conversion (kg/mg).

Equations for the movement of toxins due to pore water transport are the same whether the toxin is directly dissolved in the pore water or is carried by DOM in pore water. These equations are basically the same as the equations for the transport of DOM in pore water described earlier. As a reminder, these equations are relevant only for the active layer of the sediment system. Pore water below the active layer moves only as a result of diffusion or when a layer moves up or down one layer intact as a result of an erosional or depositional regime.

$$GainTox_{up} = (Conc_{Tox\ n-1})\ (GainPW_{up})\ \frac{AvgArea \cdot 1E3}{PoreWaterVol} \quad \textbf{(39)}$$

where:

$GainTox_{Up}$	=	gain of toxicant due to pore water gain from the layer above (mg/L_{pw}·d);
$Conc_{Tox\ -1}$	=	concentration of toxicant in above layer ($mg/L_{upper\ water}$);
$GainPW_{up}$	=	gain of pore water from above ($m^3_{upper\ water}/m^2$·d);
AvgArea	=	average area of the segment (m^2);
1 E 3	=	units conversion (L/m^3);
PoreWaterVol	=	pore water volume (L);

and

$$LossTox_{up} = Conc_{Tox\ n} \frac{LossPW_{up}}{PoreWaterConc} \quad \textbf{(40)}$$

where:

$LossTox_{Up}$	=	loss of toxicant due to pore water movement to the layer above (mg/L_{pw}·d);
$Conc_{Tox\ n}$	=	concentration of toxicant in this layer (mg/L_{pw});
$LossPW_{up}$	=	loss of pore water to above layer (m^3_{pw}/m^2·d); and
PoreWaterConc	=	pore water concentration (m^3_{pw}/m^2).

Microbial Degradation

Not only can microorganisms decompose the detrital organic material in ecosystems, they also can degrade xenobiotic organic compounds such as fuels, solvents, pesticides, and PCBs to obtain energy. In AQUATOX, this process of biodegradation of pollutants, whether they are dissolved in the water column or adsorbed to organic detritus in the water column or sediments, is modeled using the same equations as for decomposition of detritus, substituting the pollutant and its degradation parameters for detritus:

$$MicrobialDegrdn = KMDegrdn_{Phase} \cdot DOCorrection \cdot TCorr \cdot pHCorr \cdot Toxicant_{Phase} \quad \textbf{(41)}$$

where:

$MicrobialDegrdn$	=	loss due to microbial degradation ($g/m^3 \cdot d$);
$KMDegrdn_{phase}$	=	maximum degradation rate, either in water column or sediments (day^{-1});
$DOCorrection$	=	effect of anaerobic conditions (unitless);
$TCorr$	=	effect of suboptimal temperature (unitless);
$pHCorr$	=	effect of suboptimal pH (unitless); and
$Toxicant_{phase}$	=	concentration of organic toxicant in water column or sediments (g/m^3).

Volatilization

Volatilization is modeled using the "stagnant boundary theory," or two-film model, in which a pollutant molecule must diffuse across both a stagnant water layer and a stagnant air layer to volatilize out of a waterbody (Whitman, 1923; Liss and Slater, 1974). Diffusion rates of pollutants in these stagnant boundary layers can be related to the known diffusion rates of chemicals such as oxygen and water vapor. The thickness of the stagnant boundary layers must also be taken into account to estimate the volatile flux of a chemical out of (or into) the waterbody.

The time required for a pollutant to diffuse through the stagnant water layer in a waterbody is based on the well-established equations for the reaeration of oxygen, corrected for the difference in diffusivity as indicated by the respective molecular weights (Thomann and Mueller, 1987, p. 533). The diffusivity through the water film is greatly affected by the degree of ionization (Schwarzenbach et al., 1993, p. 243), and the depth-averaged reaeration coefficient is multiplied by the thickness of the well-mixed zone:

$$KLiq = KReaer \cdot Thick \cdot \left(\frac{MolWtO2}{MolWt} \right)^{0.25} \cdot \frac{1}{Nondissoc} \quad \textbf{(42)}$$

where:

$KLiq$	=	water-side transfer velocity (m/d);
$KReaer$	=	depth-averaged reaeration coefficient for oxygen (L/d);

Thick = thickness of well-mixed layer (m);
MolWtO2 = molecular weight of oxygen (g/mol, =32);
MolWt = molecular weight of pollutant (g/mol); and
Nondissoc = nondissociated fraction (unitless).

Reaeration is a function of the depth-averaged mass transfer coefficient *KReaer*, corrected for ambient temperature, multiplied by the difference between the dissolved oxygen level and the saturation level (cf. Bowie et al., 1985):

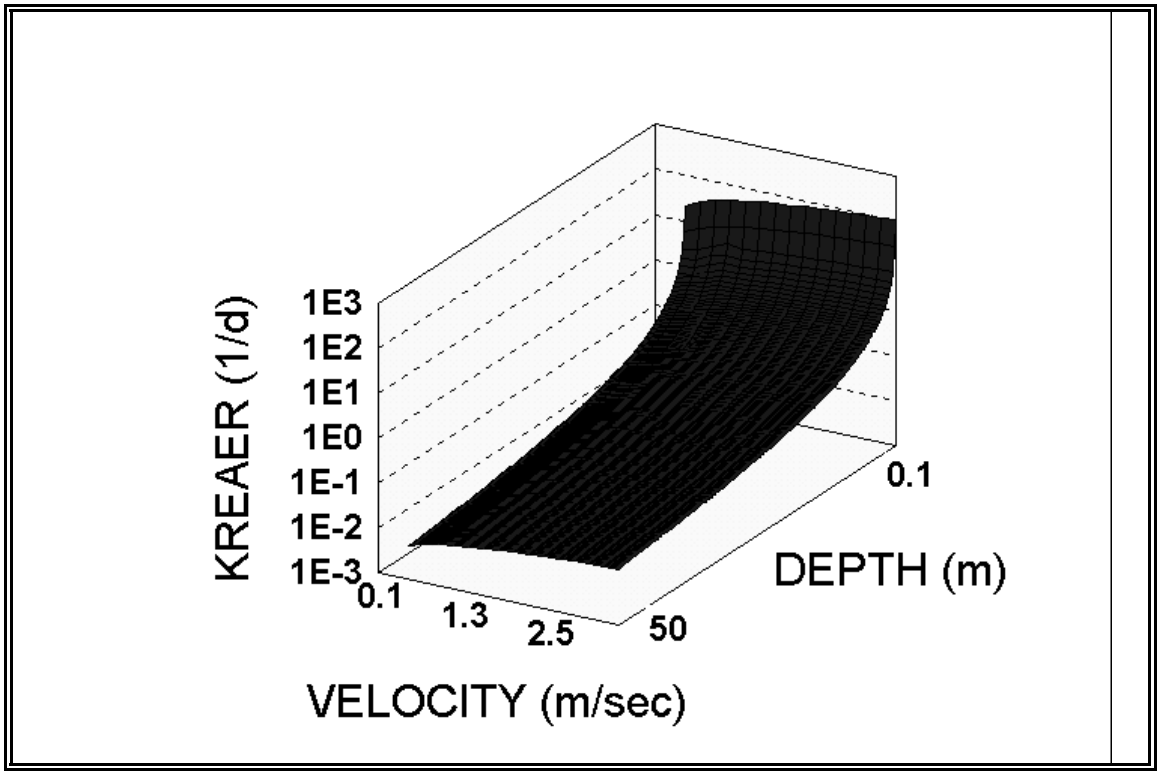
$$Reaeration = KReaer \cdot (O2Sat - Oxygen) \quad \textbf{(43)}$$

where:
Reaeration = mass transfer of oxygen ($g/m^3 \cdot d$);
KReaer = depth-averaged reaeration coefficient (L/d);
Temperature = ambient water temperature (°C);
O2Sat = saturation concentration of oxygen (g/m^3); and
Oxygen = concentration of oxygen (g/m^3).

In standing water, *KReaer* is computed as a minimum transfer velocity plus the effect of wind on the transfer velocity (Schwarzenbach et al., 1993) divided by the thickness of the mixed layer to obtain a depth-averaged coefficient.

In streams, reaeration is a function of current velocity and water depth (**Figure 8**) following the approach of Covar (1976, see Bowie et al., 1985) and used in WASP (Ambrose et al., 1991). The decision rules for which equation to use are taken from the WASP5 code (Ambrose et al., 1993).

Figure 8
Reaeration in Streams



If reaeration due to wind exceeds that due to current velocity, the equation for standing water is used; reaeration is set to 0 if there is ice cover.

To estimate the air-side transfer velocity of a pollutant, the following empirical equation, based on the evaporation of water, corrected for the difference in diffusivity of water vapor compared to the toxicant (Thomann and Mueller, 1987, p. 534), is used:

$$KGas = 168 \cdot \left(\frac{MolWtH2O}{MolWt} \right)^{0.25} \cdot Wind \qquad \textbf{(44)}$$

where:

KGas	=	air-side transfer velocity (m/d);
Wind	=	wind speed ten meters above the water surface (m/s); and
MolWtH2O	=	molecular weight of water (g/mol, =18).

The total resistance to the mass transfer of the pollutant through both the stagnant boundary layers can be expressed as the sum of the resistances—the reciprocals of the air- and water-phase mass transfer coefficients (Schwarzenbach et al., 1993), modified for the effects of ionization:

$$\frac{1}{KOVol} = \frac{1}{KLiq} + \frac{1}{KGas \cdot HenryLaw \cdot Nondissoc} \qquad \textbf{(45)}$$

where:

KOVol = total mass transfer coefficient through both stagnant boundary layers (m/d);

$$HenryLaw = \frac{Henry}{R \cdot TKelvin} \quad \textbf{(46)}$$

and where:

HenryLaw = Henry's Law constant (unitless*);*
Henry = Henry's Law constant (atm m^3 mol^{-1});
R = gas constant (=8.206E-5 atm m^3 (mol K)$^{-1}$); and
TKelvin = temperature in °K.

The Henry's law constant is applicable only to the fraction that is nondissociated because the ionized species will not be present in the gas phase (Schwarzenbach et al., 1993, p. 179).

The atmospheric exchange of the pollutant can be expressed as the depth-averaged total mass transfer coefficient times the difference between the concentration of the chemical and the saturation concentration:

$$Volatilization = \frac{KOVol}{Thick} \cdot \left(ToxSat - Toxicant_{water}\right) \quad \textbf{(47)}$$

where:

Volatilization = interchange with atmosphere (µg/L·d);
Thick = depth of water or thickness of surface layer (m);
ToxSat = saturation concentration of pollutant (µg/L); and
$Toxicant_{water}$ = concentration of pollutant in water (µg/L).

The saturation concentration depends on the concentration of the pollutant in the air, ignoring temperature effects (Thomann and Mueller, 1987, p. 532), but adjusting for ionization and units:

$$ToxSat = \frac{Toxicant_{air}}{HenryLaw \cdot Nondissoc} \cdot 1000 \quad \textbf{(48)}$$

where:

$Toxicant_{air}$ = gas-phase concentration of the pollutant (g/m^3); and
Nondissoc = nondissociated fraction (unitless).

Often the pollutant can be assumed to have a negligible concentration in the air and *ToxSat* is zero. However, this general construct can represent the transferral of volatile pollutants into water bodies. Because ionized species do not volatilize, the saturation level increases if ionization is occurring.

The nondimensional Henry's law constant, which relates the concentration of a compound in the air phase to its concentration in the water phase, strongly affects the air-phase resistance. Depending on the value of the Henry's law constant, the water phase, the air phase, or both may control volatilization.

Partition Coefficients

Although AQUATOX is a kinetic model, steady-state partition coefficients for organic pollutants are computed to place constraints on competitive uptake and loss processes, speeding up computations. They can be supplied by the user or estimated from empirical regression equations and the octanol-water partition coefficient for the contaminant.

Natural organic matter is the primary sorbent for neutral organic pollutants. Hydrophobic chemicals partition primarily in nonpolar organic matter (Abbott et al., 1995). Most detritus is relatively nonpolar; its partition coefficient is a function of the octanol-water partition coefficient (N = 34, r^2 = 0.93; Schwarzenbach et al. 1993):

$$KOM_{Detr} = 1.38 \cdot KOW^{0.82} \quad \textbf{(49)}$$

where:

KOM_{Detr} = detritus-water partition coefficient (L/kg); and
KOW = octanol-water partition coefficient (unitless).

O'Connor and Connolly (1980); (see also Ambrose et al., 1991) found that the sediment partition coefficient is the inverse of the mass of suspended sediment. Di Toro (1985) developed a construct to represent the relationship. This may be an artifact due to complexation with dissolved and colloidal organics (Schnoor, 1996); therefore, the partition coefficient is not corrected for mass of sediment.

Association of hydrophobic compounds with colloidal and dissolved organic matter (DOM) reduces bioavailability; such contaminants are unavailable for uptake by organisms (Stange and Swackhamer, 1994; Gilek et al., 1996). Therefore, it is important that complexation of organic chemicals with DOM be modeled. Analysis of data from a study using naturally occurring fulvic acids (Uhle et al., 1999) exhibits a relationship between these two parameters (**Figure 9**; N = 3, r^2 = 0.76). Although additional points would be preferable, the relationship is consistent with other lines of evidence (see below); therefore, it is used as the default estimator to represent complexation with DOM in AQUATOX:

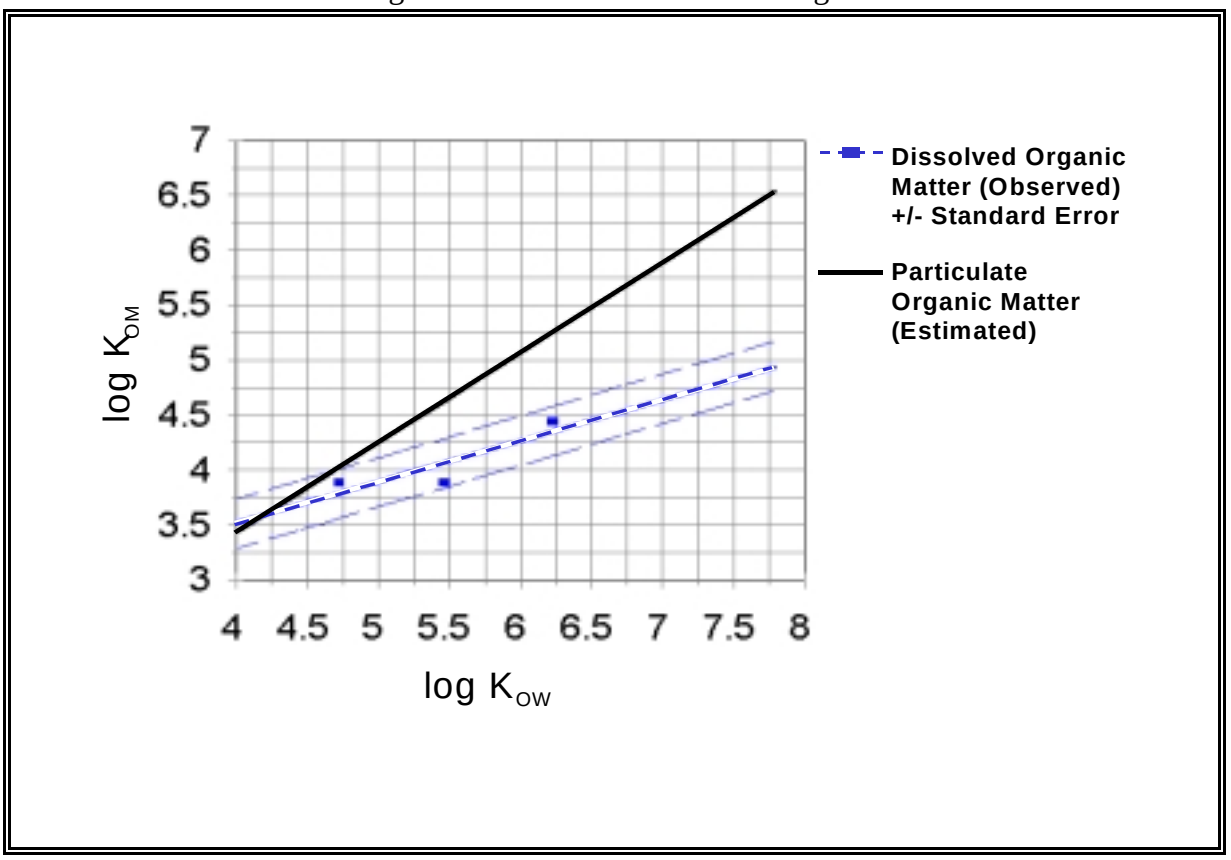
$$KOM_{DOM} = 190 \cdot KOW^{0.38} \cdot 0.526 \quad \textbf{(50)}$$

where:

KOM_{DOM} = partition coefficient for dissolved organic matter (L/kg);
0.526 = factor to convert from organic carbon to organic matter.

Comparing the results of using these coefficients, we see that they are consistent with the relative importance of the forms of detritus in binding organic chemicals (**Figure 9**). Binding capacity of particulate detritus is greater than dissolved organic matter in Great Lakes waters (Stange and Swackhamer, 1994; Gilek et al., 1996). In a study using Baltic Sea water, less than 7% of the mass of PCBs was associated with dissolved organic matter and most of the mass was associated with algae (Björk and Gilek, 1999). Analysis of PCB data from the Hudson River indicated that partitioning to dissolved organic matter was a significant component for Cl_1 and Cl_2 PCBs, but not for more chlorinated congeners; however, a three-component model may still be advisable to avoid overestimating bioavailability (Butcher et al., 1998).

Figure 9
Partitioning to Dissolved and Particulate Organic Matter



Older data and modeling efforts failed to distinguish between hydrophobic compounds that were truly dissolved and those that were complexed with DOM. For example, the PCB water concentrations for Lake Ontario, reported by Oliver and Niimi (1988) and used by many subsequent researchers, included both dissolved and DOC-complexed PCBs (a fact which they recognized). In their steady-state model of PCBs in the Great Lakes, Thomann and Mueller (1983) defined "dissolved" as that which is not particulate (passing a 0.45-micron filter). In their Hudson River PCB model, Thomann et al. (1991) again used an operational definition of dissolved PCBs. AQUATOX models truly dissolved and complexed compounds separately, but offers the analyst the

option of calculating apparent partitioning factors using either definition of "dissolved," facilitating comparison with observed data.

Bioaccumulation of PCBs in algae depends on solubility; hydrophobicity and molecular configuration of the compound, growth rate, surface area and type, and content and type of lipid in the algae (Stange and Swackhamer, 1994). Phytoplankton biomass may double or triple in one day and periphyton turnover may be so rapid that some PCBs will not reach equilibrium (Hill and Napolitano, 1997); therefore, one should use the term "bioaccumulation factor" (BAF) rather than "bioconcentration factor," which implies equilibrium (Stange and Swackhamer, 1994). Algal lipids have a much stronger affinity for hydrophobic compounds than does octanol, so that the algal $BAF_{lipid} > K_{OW}$ (Stange and Swackhamer, 1994; Koelmans et al., 1995; Sijm et al., 1998).

For phytoplankton, the approximation to estimate the dry-weight bioaccumulation factor ($r^2 = 0.87$), computed from Swackhamer and Skoglund's (1993) study of approximately 52 PCB congeners, is:

$$\log(BAF_{Alga}) = 0.41 + 0.91 \cdot \log K_{OW} \quad \textbf{(51)}$$

where:

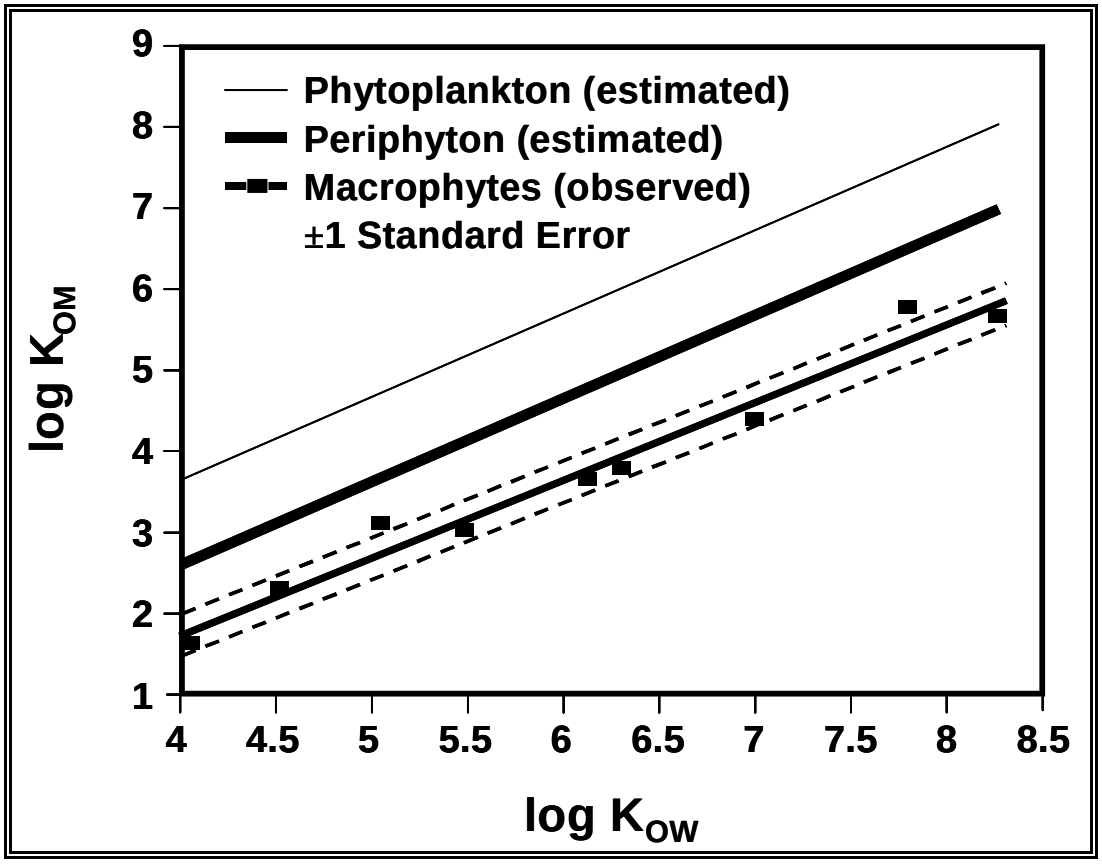
BAF_{Alga} = partition coefficient between algae and water (L/kg).

For macrophytes, an empirical relationship reported by Gobas et al. (1991) for nine chemicals with $logK_{OW}$s of 4 to 8.3 ($r^2 = 0.97$) is used:

$$\log(BAF_{Macro}) = 0.98 \cdot \log K_{OW} - 2.24 \quad \textbf{(52)}$$

Periphyton bioconcentration factors are an order of magnitude less than those for phytoplankton (Wang et al., 1999), and this relationship is used to estimate the partition coefficients in AQUATOX (**Figure 10**).

Figure 10
Partitioning to Various Types of Plants



For the invertebrate partition coefficient, if the user does not supply a value, the following empirical equation is used, based on seven chemicals with log K_{OW}s ranging from 3.3 to 6.2 and bioaccumulation factors for *Daphnia pulex* (r^2 = 0.85; Southworth et al., 1978; see also Lyman et al., 1982), converted to dry weight :

$$\log(KB_{Invertebrate}) = (0.7520 \cdot \log K_{OW} - 0.4362) \cdot WetToDry \quad \textbf{(53)}$$

where:

$KB_{Invertebrate}$ = partition coefficient between invertebrates and water (L/kg); and
WetToDry = wet to dry conversion factor (unitless, default = 5).

Fish take longer to reach equilibrium with the surrounding water; therefore, a nonequilibrium bioconcentration factor is used. For each pollutant, a whole-fish bioconcentration factor is based on the lipid content of the fish extended to hydrophilic chemicals (McCarty et al., 1992), with provision for ionization:

$$KB_{Fish} = 1 + Lipid \cdot WetToDry \cdot K_{OW} \quad \textbf{(54)}$$

where:

KB_{Fish}	=	partition coefficient between whole fish and water (L/kg);
Lipid	=	fraction of fish that is lipid (g lipid/g fish); and
WetToDry	=	wet to dry conversion factor (unitless, default = 5).

Lipid content of fish can be fixed by the modeler or can be varied depending on the potential for growth as predicted by the bioenergetics equations; the initial lipid values for each species are given. The bioconcentration factor is adjusted for the time to reach equilibrium as a function of the clearance or elimination rate and the time of exposure (Hawker and Connell, 1985; Connell and Hawker, 1988; **Figure 11**):

$$BCF_{Fish} = KB_{Fish} \cdot \left(1 - e^{(-Elimination \cdot TElapsed)}\right) \quad \textbf{(55)}$$

where:

BCF_{Fish}	=	quasi-equilibrium bioconcentration factor for fish (L/kg);
TElapsed	=	time elapsed since fish was first exposed (d); and
Elimination	=	combined clearance and biotransformation.

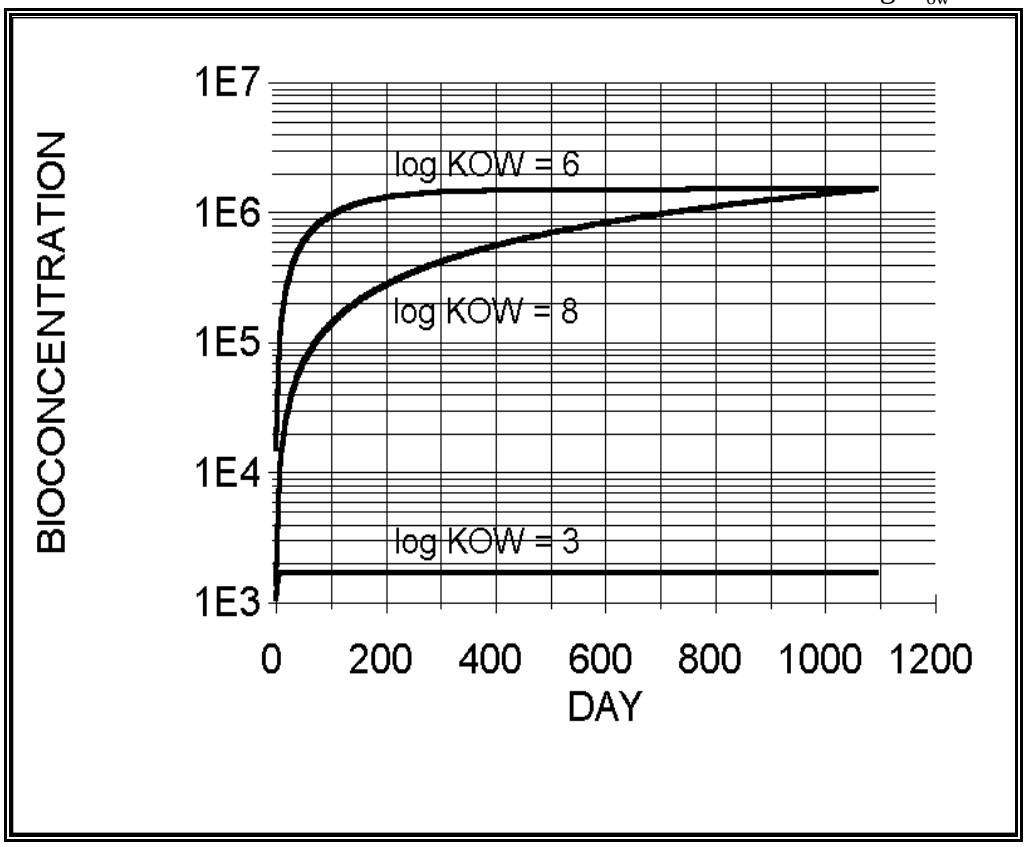
The concentration in each carrier is given by:

$$PPB_i = \frac{ToxState_i}{CarrierState_i} \cdot 1E6 \quad \textbf{(56)}$$

where:

PPB_i	=	concentration of chemical in carrier *i* (µg/kg);
$ToxState_i$	=	mass of chemical in carrier *i* (ug/L);
CarrierState	=	biomass of carrier (mg/L); and
1E6	=	conversion factor (mg/kg).

Figure 11
Bioconcentration Factor for Fish as a Function of Time and Log K_{ow}



Nonequilibrium Kinetics

Often there is an absence of equilibrium due to growth or insufficient exposure time, metabolic biotransformation, dietary exposure, and nonlinear relationships for very large and/or superhydrophobic compounds (Bertelsen et al., 1998). Although it is important to have a knowledge of equilibrium partitioning because it is an indication of the condition toward which systems tend (Bertelsen et al., 1998), it is often impossible to determine steady-state potential due to changes in bioavailability and physiology (Landrum, 1998). For example, PCBs may not be at steady state even in large systems such as Lake Ontario that have been polluted over a long period of time. In fact, PCBs in Lake Ontario exhibit a 25-fold disequilibrium (Cook and Burkhard, 1998).

Sorption and Desorption to Sedimented Detritus

Partitioning to sediments appears to involve rapid sorption to particle surfaces, followed by slow movement into, and out of, organic matter and porous aggregates (Karickhoff and Morris, 1985). Therefore, attainment of equilibrium may be slow. This applies to suspended detritus compartments as well. Because of the need to represent sorption and desorption separately in detritus, kinetic formulations are used (Thomann and Mueller, 1987):

$$Sorption = k1_{Detr} \cdot Toxicant_{Water} \cdot Diff1_{Carrier} \cdot Org2C \cdot Detr \cdot 1E-6 \quad \textbf{(57)}$$

$$Desorption = k2_{Detr} \cdot Diff2_{Carrier} \cdot Toxicant_{Detr} \quad \textbf{(58)}$$

where:

Sorption	=	rate of sorption to given detritus compartment (μg/L·d);
$k1_{Detr}$	=	sorption rate constant (L/kg·d);
$Toxicant_{Water}$	=	concentration of toxicant in water (μg/L);
$Diff1_{Carrier}$	=	factor to normalize rate constant for given carrier (detritus compartment in this case) based on all competing uptake rates (unitless);
$Diff2_{Carrier}$	=	factor to normalize loss rates (unitless);
Org2C	=	conversion factor for organic matter to carbon (= 0.526 g C/g organic matter);
Detr	=	mass of each of the detritus compartments per unit volume (mg/L);
1e -6	=	units conversion (kg/mg);
Desorption	=	rate of desorption from given sediment detritus compartment (μg/L·d);
$k2_{Detr}$	=	desorption rate constant (day^{-1}); and
$Toxicant_{Detr}$	=	mass of toxicant in each of the detritus compartments (μg/L).

Because there are several processes competing for the dissolved toxicant, the rate constants for these processes are normalized to preserve mass balance. The *Diff1* factor is computed for each direct uptake process, including sorption to detritus and algae, uptake by macrophytes, and uptake across animals' gills:

$$RateDiff1_{Carrier} = Gradient1_{Carrier} \cdot k1 \quad \textbf{(59)}$$

$$Gradient1_{Carrier} = \frac{Toxicant_{Water} \cdot kp_{Carrier} - PPB_{Carrier}}{Toxicant_{Water} \cdot kp_{Carrier}} \quad \textbf{(60)}$$

$$Diff1_{Carrier} = \frac{RateDiff_{Carrier}}{\sum RateDiff_{Carrier}} \quad \textbf{(61)}$$

where:

$RateDiff1_{Carrier}$ = maximum rate constant for uptake given the concentration gradient (L/kg·d);

$Gradient1_{Carrier}$ = gradient between potential and actual concentrations of toxicant in each carrier (unitless);

$kp_{Carrier}$ = partition coefficient or bioconcentration factor for each carrier (L/kg); and

$PPB_{Carrier}$ = concentration of toxicant in each carrier (µg/kg).

Likewise, the loss rate constants are normalized; the equations parallel those for uptake, with the gradient being reversed:

$$RateDiff2_{Carrier} = Gradient2_{Carrier} \cdot k2 \quad \textbf{(62)}$$

$$Gradient2_{Carrier} = \frac{PPB_{Carrier} - (PPB_{Water} \cdot kp_{Carrier})}{PPB_{Carrier}} \quad \textbf{(63)}$$

$$Diff2_{Carrier} = \frac{RateDiff2_{Carrier}}{\sum RateDiff2_{Carrier}} \quad \textbf{(64)}$$

where:

$RateDiff2_{Carrier}$ = maximum rate constant for loss given the concentration gradient (L/kg·d); and

$Gradient2_{Carrier}$ = gradient between actual and potential concentrations of toxicant in each carrier (unitless).

Desorption of the slow compartment is the reciprocal of the reaction time, which Karickhoff and Morris (1985) found to be a linear function of the partition coefficient over three orders of magnitude ($r^2 = 0.87$):

$$\frac{1}{k2} \approx 0.03 \cdot 24 \cdot KPSed \quad \textbf{(65)}$$

So *k2* is taken to be:

$$k2 = \frac{1.39}{KPSed} \quad \textbf{(66)}$$

where:

KPSed = detritus-water partition coefficient (L/kg); and
24 = conversion from hours to days.

The slow compartment may be involved in 40 to 90% of the desorption so, as a simplification, fast desorption of the labile compartment is ignored. The sorption rate constant *k1* is set to 1200 L/kg·d, representing the very fast sorption of most chemicals. Alternative formulations recognizing both fast and slow sorption and desorption are still being evaluated.

Bioconcentration in Macrophytes and Algae

Macrophytes—As Gobas et al. (1991) have shown, submerged aquatic macrophytes take up and release organic chemicals over a measurable period of time at rates related to the octanol-water partition coefficient. Uptake and elimination are modeled assuming that the chemical is transported through both aqueous and lipid phases in the plant, with rate constants using empirical equations fit to observed data (Gobas et al., 1991), modified to account for ionization effects (**Figure 12**, **Figure 13**):

$$MacroUptake = k1 \cdot Diff1_{Plant} \cdot Toxicant_{Water} \cdot StVar_{Plant} \cdot 1E-6 \quad \textbf{(67)}$$

$$Depuration_{Plant} = k2 \cdot Toxicant_{Plant} \cdot Diff2_{Plant} \quad \textbf{(68)}$$

$$k1 = \frac{1}{0.0020 + \frac{500}{KOW \cdot Nondissoc}} \quad \textbf{(69)}$$

$$k2 = \frac{1}{1.58 + 0.000015 \cdot KOW \cdot Nondissoc} \quad \textbf{(70)}$$

where:

MacroUptake = uptake of toxicant by plant (µg/L·d);
$Depuration_{Plant}$ = clearance of toxicant from plant (µg/L·d);
$StVar_{Plant}$ = biomass of given plant (mg/L);
1 E -6 = units conversion (kg/mg);
$Toxicant_{Plant}$ = mass of toxicant in plant (µg/L);
k1 = sorption rate constant (L/kg·d);
k2 = elimination rate constant (1/d);
$Diff1_{Plant}$ = factor to normalize uptake rates (unitless);
$Diff2_{Plant}$ = factor to normalize loss rates (unitless);
KOW = octanol-water partition coefficient (unitless); and

Nondissoc = fraction of un-ionized toxicant (unitless).

Figure 12
Uptake Rate Constant for Macrophytes
(after Gobas et al., 1991)

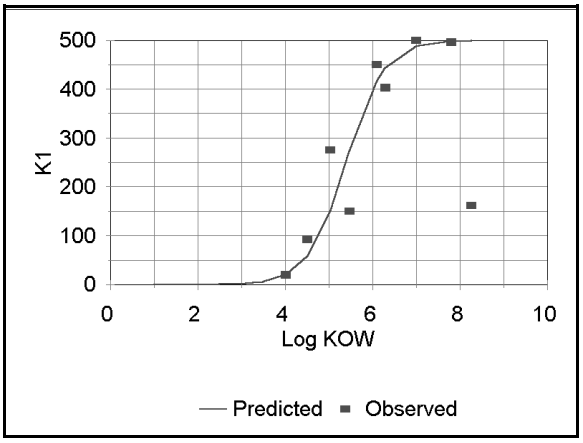
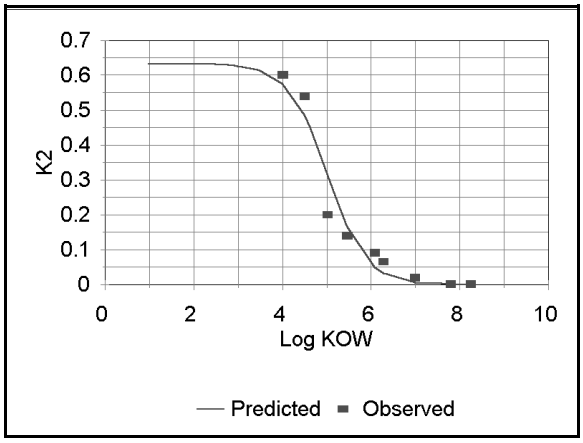


Figure 13
Elimination Rate Constant for Macrophytes
(after Gobas et al., 1991)



Algae—There is probably a two-step algal bioaccumulation mechanism for hydrophobic compounds, with rapid surface sorption of 40-90% of the compound within 24 hours and then a small, steady increase with transfer to interior lipids for the duration of the exposure (Swackhamer and Skoglund, 1991). Uptake increases with increase in the relative surface area of algae (Wang et al., 1997). Therefore, the smaller the organism the larger the uptake rate constant (Sijm et al., 1998). However, in small phytoplankton, such as the nannoplankton that dominate the Great Lakes, a high surface to volume ratio can increase sorption, but high growth rates can limit internal contaminant concentrations (Swackhamer and Skoglund, 1993). The combination of lipid content, surface area, and growth rate results in species differences in bioaccumulation factors among algae (Wood et al., 1997). Uptake of toxicants is a function of the uptake rate constant and the concentration of toxicant truly dissolved in the water, and is constrained by competitive uptake by other compartments:

$$AlgalUptake = k1 \cdot Michaelis \cdot Diff1 \cdot ToxState \cdot Carrier \cdot 1E-6 \qquad \textbf{(71)}$$

where:

AlgalUptake = rate of sorption by algae (µg/L·d);
k1 = uptake rate constant (L/kg·d), see **(72)**;
Michaelis = Michaelis-Menten construct for nonlinear uptake (unitless), see **(73)**;
Diff1 = factor to normalize uptake rates (unitless), see **(59)**;
ToxState = concentration of dissolved toxicant (µg/L);
Carrier = biomass of algal compartment (mg/L); and
1E-6 = conversion factor (kg/mg).

The kinetics of partitioning of toxicants to algae is based on studies on PCB congeners in The Netherlands by Koelmans, Sijm, and colleagues and at the University of Minnesota by Skoglund and Swackhamer. Both groups found uptake to be very rapid. Sijm et al. (1998) presented data on several congeners that were used in this study to develop the following relationship for phytoplankton (**Figure 14**):

$$k1 = \frac{1}{1.8\text{E}-6 + 1/(K_{OW} \cdot Nondissoc)} \quad \textbf{(72)}$$

Because size-dependent passive transport is indicated (Sijm et al., 1998) and the bioaccumulation factor for periphyton has been found to be an order of magnitude less than that for phytoplankton (Wang et al.,1999), uptake by periphyton is set at 10% of that for phytoplankton.

To represent saturation kinetics, *Michaelis* is computed as:

$$Michaelis = \frac{BCF_{Algae} \cdot ToxState - PPB_{Algae}}{BCF_{Algae} \cdot ToxState} \quad \textbf{(73)}$$

where:

BCF_{Algae} = steady-state bioconcentration factor for algae (L/kg); and
PPB_{Algae} = concentration of toxicant in algae (mg/kg).

Depuration is modeled as a linear function; it does not include loss due to excretion of photosynthate with associated toxicant, which is modeled separately.

$$Depuration = k2 \cdot State \quad \textbf{(74)}$$

where:

Depuration = elimination of toxicant (µg/L·d);
State = concentration of toxicant associated with alga (µg/L); and
k2 = elimination rate constant (day^{-1}).

Based in part on Skoglund et al. (1996), but ignoring surface sorption and recognizing that growth dilution is explicit in AQUATOX, the elimination rate constant (**Figure 15**) is computed as:

$$k2 = \frac{k1}{K_{OW}} \quad \textbf{(75)}$$

Aside from obvious structural differences, algae may have very high lipid content (20% for *Chlorella* sp. according to Jørgensen et al., 1979) and macrophytes have a very low lipid content (0.2% in *Myriophyllum spicatum* as observed by Gobas et al., 1991), which affect both uptake and elimination of toxicants. The uptake rate for macrophytes is much less than for phytoplankton, but in a shallow-water system, such as parts of the Housatonic River, very high macrophyte biomass may constitute a large seasonal sink for PCBs.

Figure 14
Algal Sorption Rate Constant as a Function of Octanol-Water Partition Coefficient

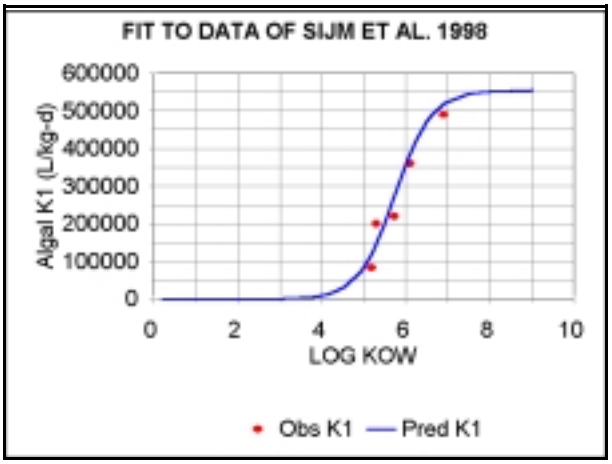
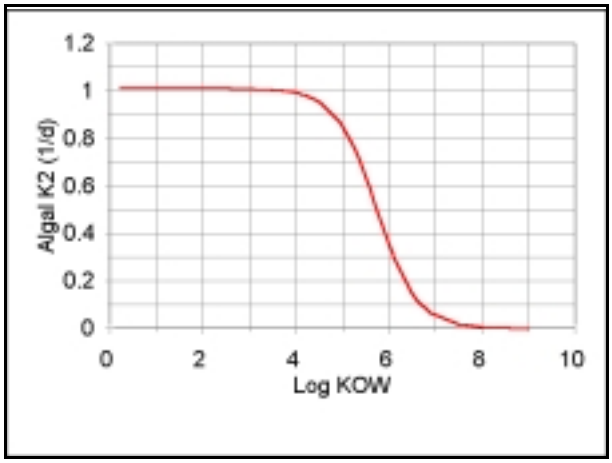


Figure 15
Rate of Elimination by Algae as a Function of Octanol-Water Partition Coefficient



Bioaccumulation in Animals

Animals can absorb toxic organic chemicals directly from the water through their gills and from contaminated food through their guts. Direct sorption onto the body is ignored as a simplifying assumption in this version of the model. Reduction of body burdens of organic chemicals is accomplished through excretion and biotransformation, which are often considered together as empirically determined elimination rates. "Growth dilution" occurs when growth of the organism is faster than accumulation of the toxicant. Gobas (1993) includes fecal egestion, but in AQUATOX egestion is merely the amount ingested but not assimilated; it is accounted for indirectly in *DietUptake*. However, fecal loss is important as an input to the detrital toxicant pool, and it is considered below in that context. Inclusion of mortality and promotion terms is necessary for mass balance, but emphasizes the fact that average concentrations are being modeled for any particular compartment.

Gill Sorption—Active transport through the gills is an important route of exposure (Macek et al., 1977). This is the route that has been measured so often in bioconcentration experiments with fish. As the organism respires, water is passed over the outer surface of the gill and blood is moved past the inner surface. The exchange of toxicant through the gill membrane is assumed to be facilitated by the same mechanism as the uptake of oxygen, following the approach of Fagerström and Åsell (1973, 1975), Weininger (1978), and Thomann and Mueller (1987; see also Thomann, 1989). Therefore, the uptake rate for each animal can be calculated as a function of respiration (Leung, 1978; Park, Connolly, et al., 1980):

$$KUptake = \frac{WEffTox \cdot Respiration \cdot O2Biomass}{Oxygen \cdot WEffO2} \qquad \textbf{(76)}$$

$$GillUptake = KUptake \cdot Toxicant_{Water} \cdot Diff1_{Carrier} \quad \textbf{(77)}$$

where:

GillUptake	=	uptake of toxicant by gills (μg/L·d);
KUptake	=	uptake rate (day^{-1});
$Toxicant_{Water}$	=	concentration of toxicant in water (μg/L);
$Diff1_{Carrier}$	=	factor to normalize rate constant for given carrier (animal compartment in this case) based on all competing uptake rates (unitless), see **(59)**;
WEffTox	=	withdrawal efficiency for toxicant by gills (unitless), see **(78)**;
Respiration	=	respiration rate (mg biomass/L·d);
O2Biomass	=	ratio of oxygen to organic matter (mg oxygen/mg biomass; generally 0.575);
Oxygen	=	concentration of dissolved oxygen (mg oxygen/L); and
WEffO2	=	withdrawal efficiency for oxygen (unitless, generally 0.62).

The oxygen uptake efficiency *WEffO2* is assigned a constant value of 0.62 based on observations of McKim et al. (1985). The toxicant uptake efficiency, *WEffTox*, can be expected to have a sigmoidal relationship to the log K_{ow} based on aqueous and lipid transport (Spacie and Hamelink, 1982). This is represented by a piece-wise fit (**Figure 16**) to the data of McKim et al. (1985) using 750-g fish, corrected for ionization:

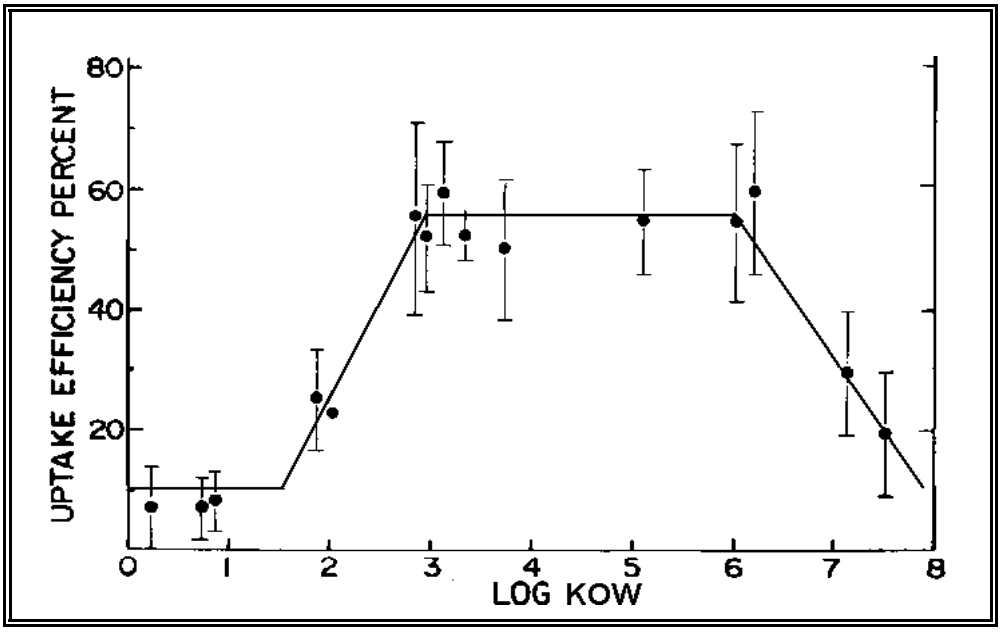
$$\begin{gathered}
\text{If } \log K_{OW} < 1.5 \text{ then} \\
WEffTox = 0.1 \\
\\
\text{If } 1.5 \le \log K_{OW} > 3.0 \text{ then} \\
WEffTox = 0.1 + Nondissoc \cdot (0.3 \cdot LogKOW - 0.45) \\
\\
\text{If } 3.0 \le \log K_{OW} \le 6.0 \text{ then} \\
WEffTox = 0.1 + Nondissoc \cdot 0.45 \\
\\
\text{If } 6.0 < \log K_{OW} < 8.0 \text{ then} \\
WEffTox = 0.1 + Nondissoc \cdot (0.45 - 0.23 \cdot (LogKOW - 6.0)) \\
\\
\text{If } \log K_{OW} \ge 8.0 \text{ then} \\
WEffTox = 0.1
\end{gathered} \quad \textbf{(78)}$$

where:

LogKOW	=	log octanol-water partition coefficient (unitless); and
Nondissoc	=	fraction of toxicant that is un-ionized (unitless).

This same algorithm is used for invertebrates. Thomann (1989) has proposed a similar construct for these same data and a slightly different construct for small organisms, but the scatter in the data does not seem to justify using two different constructs.

Figure 16
Piece-Wise Fit to Observed Toxicant Uptake Data;
Modified from McKim et al., 1985



Dietary Uptake—Hydrophobic chemicals usually bioaccumulate primarily through absorption from contaminated food. Persistent, highly hydrophobic chemicals demonstrate biomagnification or increasing concentrations as they are passed up the food chain from one trophic level to another; therefore, dietary exposure can be quite important (Gobas et al., 1993). Uptake from contaminated prey can be computed as (Thomann and Mueller, 1987; Gobas, 1993):

$$DietUptake_{Prey} = KD_{Prey} \cdot PPB_{Prey} \cdot 1E-6 \quad \textbf{(79)}$$

$$KD_{Prey} = GutEffTox \cdot Ingestion_{Prey} \quad \textbf{(80)}$$

where:

$DietUptake_{Prey}$	=	uptake of toxicant from given prey (μg toxicant/L·d);
KD_{Prey}	=	dietary uptake rate for given prey (mg prey/L·d);
PPB_{Prey}	=	concentration of toxicant in given prey (μg toxicant/kg prey);
1 E-6	=	units conversion (kg/mg);
GutEffTox	=	efficiency of sorption of toxicant from gut (unitless); and

$Ingestion_{Prey}$ = ingestion of given prey (mg prey/L·d).

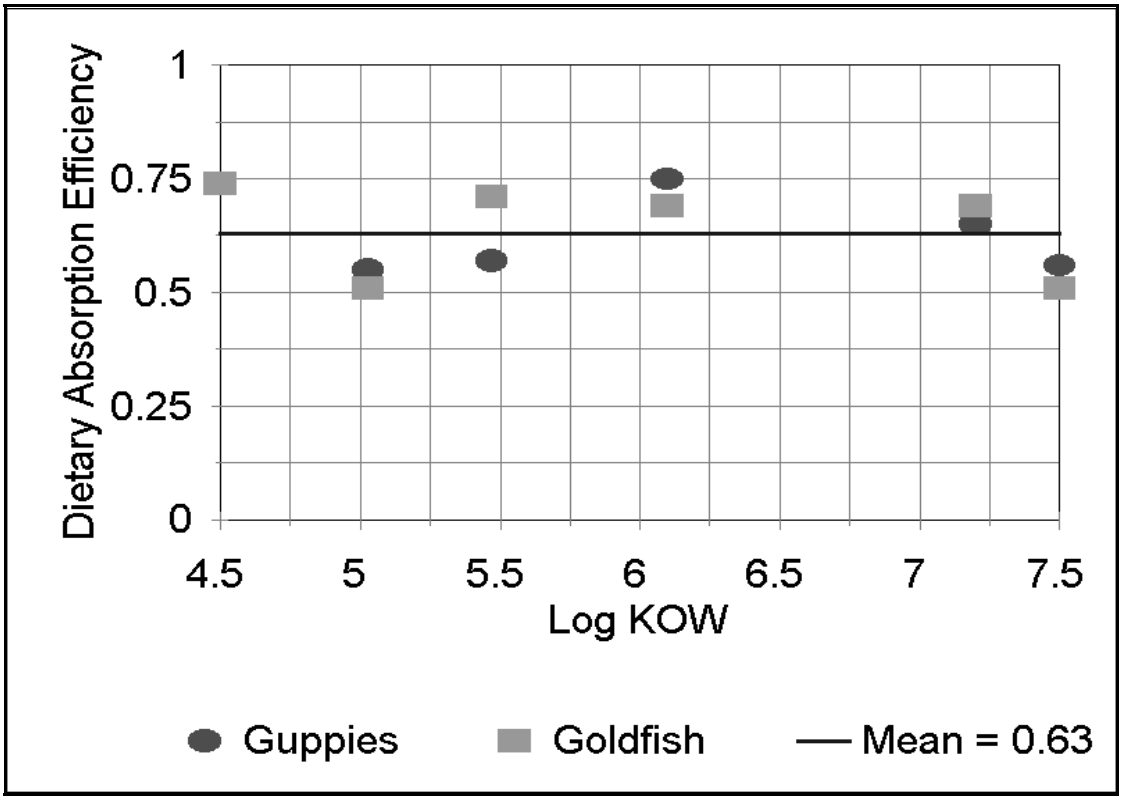
Data published by Gobas et al. (1993) suggest that there is no trend in efficiency for chemicals with log K_{OW} between 4.5 and 7.5 (**Figure 17**); this is to be expected because the digestive system has evolved to assimilate a wide variety of organic molecules. Nichols et al. (1998) demonstrated that uptake is more efficient in larger fish; this could be a function of higher quality food. Invertebrates generally exhibit lower efficiencies; Landrum and Robbins (1990) showed that values ranged from 0.42 to 0.24 for chemicals with log K_{OW}s from 4.4 to 6.7. It appears that assimilation of lipophilic chemicals follows the assimilation of lipids (van Veld, 1990). Therefore, AQUATOX uses the same assimilation efficiency for contaminant as for food, similar to the approach taken in a bioaccumulation model for PCBs in the Upper Hudson River (QEA, 1999):

$$GutEffTox = 1 - Egest \quad \textbf{(81)}$$

where:

Egest = portion of ingested food not assimilated (unitless).

Figure 17
Efficiency of Uptake, Data from Gobas et al., 1993



Elimination—Elimination or clearance includes both excretion (depuration) and biotransformation of a contaminant by organisms. Biotransformation may cause underestimation of elimination

(McCarty et al., 1992). An overall elimination rate constant, based on a fit to laboratory data, is estimated for both invertebrates and fish. The user may enter both a biotransformation rate constant and a depuration rate constant based on observed data or may accept the estimate for a given organism and contaminant.

The estimation procedure is based on a slope related to log K_{OW} and an intercept that is a direct function of respiration, assuming an allometric relationship between respiration and the weight of the animal (Thomann, 1989), and an inverse function of the lipid content:

$$\text{Log } k2 = -0.536 \cdot \log K_{OW} + 0.116 \cdot \frac{WetWt^{-0.2}}{LipidFrac} \quad \textbf{(82)}$$

where:

k2	=	elimination rate constant (day^{-1}); and
KOW	=	octanol-water partition coefficient (unitless);
WetWt	=	mean wet weight of organism (g);
LipidFrac	=	fraction of lipid in organism (g lipid/g organism, dry weight);

This function is used in AQUATOX to estimate the elimination rate constant for both invertebrates and fish (**Figure 18**).

For any given time period, the clearance rate is:

$$Depuration_{Animal} = k2 \cdot Toxicant_{Animal} \quad \textbf{(83)}$$

where:

$Depuration_{Animal}$	=	clearance rate (µg/L·d); and
$Toxicant_{Animal}$	=	mass of toxicant in given animal (µg/L).

Biotransformation is modeled as:

$$Biotransformation = Toxicant_{Organism} \cdot BioRateConst \quad \textbf{(84)}$$

where:

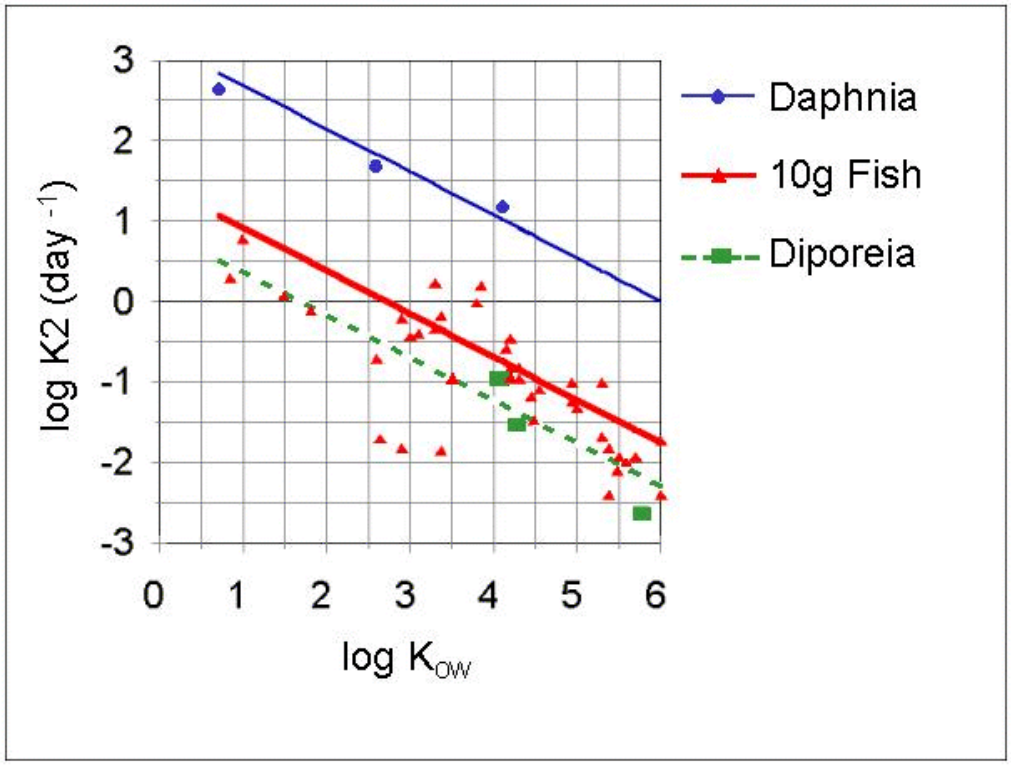
Biotransformation	=	rate of conversion of chemical by organism (µg/L·d); and
BioRateConst	=	biotransformation rate constant (day^{-1}).

Linkages to Detrital Compartments

Toxicants are transferred from organismal to detrital compartments through defecation and mortality. The amount transferred due to defecation is the unassimilated portion of the toxicant that is ingested:

$$DefecationTox = \sum (KEgest_{Pred,\ Prey} \cdot PPB_{Prey} \cdot 1E-6) \quad \textbf{(85)}$$

Figure 18
Depuration Rate Constants for Zooplankton (Daphnia), 10-g Fish, and Amphipods (Diporeia)



$$KEgest_{Pred,\ Prey} = (1 - GutEffTox) \cdot Ingestion_{Pred,\ Prey} \quad \textbf{(86)}$$

where:

$DefecationTox$	=	rate of transfer of toxicant due to defecation (µg/L·d);
$KEgest_{Pred,\ Prey}$	=	fecal egestion rate for given prey by given predator (mg prey/L·d);
PPB_{Prey}	=	concentration of toxicant in given prey (µg/kg);
1 E-6	=	units conversion (kg/mg);
$GutEffTox$	=	efficiency of sorption of toxicant from gut (unitless); and
$Ingestion_{Pred,\ Prey}$	=	rate of ingestion of given prey by given predator (mg/L·d).

The amount of toxicant transferred due to mortality may be large; it is a function of the concentrations of toxicant in the dying organisms and the mortality rates:

$$MortTox = \sum (Mortality_{Org} \cdot PPB_{Org} \cdot 1E{-}6) \quad \textbf{(87)}$$

where:

MortTox	=	rate of transfer of toxicant due to mortality (μg/L·d);
$Mortality_{Org}$	=	rate of mortality of given organism (mg/L·d);
PPB_{Org}	=	concentration of toxicant in given organism (μg/kg); and
1 E-6	=	units conversion (kg/mg).

ECOTOXICOLOGY

Toxicity can be modeled if desired; however, we do not anticipate modeling PCB toxicity in the Housatonic River project. When modeled, toxicity is based on the internal concentration of the toxicant in the specified organism. Many compounds, especially those with higher octanol-water partition coefficients, take appreciable time to accumulate in tissue. Therefore, length of exposure is critical in determining toxicity and is modeled following Mancini (1983); (see also Crommentuijn et al., 1994). The fraction killed by a given internal concentration of toxicant is estimated using the cumulative form of the Weibull distribution (Christensen and Nyholm, 1984; Mackay et al., 1992).

Organisms usually have adverse reactions to toxicants at levels significantly below those that cause death; in fact, the acute to chronic ratio is commonly used to quantify this relationship. Default application factors, which are the inverse of the acute to chronic ratio, are employed in the model to estimate chronic effect parameters. These can be supplied by the user or the default of 0.10 reported by McCarty et al. (1992) can be used.

Similar to acute toxicity, chronic toxicity is based on internal concentrations of a toxicant. The simplifying assumption is that chronic effects form a continuum with acute effects and that the difference is merely one of degree (McCarty et al., 1992). Because AQUATOX simulates biomass, no distinction is made between reduction in a process in an individual and the fraction of the population exhibiting that response. The commonly measured reduction in photosynthesis is a good example: the data indicate only that a given reduction takes place at a given concentration, not whether all individuals are affected. This approach permits efficient computation of chronic effect factors in conjunction with computation of acute effects.

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APPENDIX D.2

AQUATOX PARAMETER LIST

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AQUATOX Parameter List

Internal to AQUATOX	Tech Doc Reference	Description	Units	Data Source
ChemicalRecord	**Chemical Underlying Data**	***For each Chemical Simulated, the following parameters are required***		
ChemName	N / A	Chemical's Name. Used for Reference only.	N / A	
CASRegNo	N / A	CAS Registry Number. Used for Reference only.	N / A	
MolWt	MolWt	molecular weight of pollutant	(g/mol)	lit
Solubility	N / A	Not utilized as a parameter by the code.	(ppm)	
Henry	Henry	Henry's law constant	(atm m^3 mol^{-1})	lit & est
pka	pKa	acid dissociation constant	negative log	NA
VPress	N / A	Not utilized as a parameter by the code.	mm Hg	
LogP	LogKow	log octanol-water partition coefficient	(unitless)	lit
En	En	Arrhenius activation energy	(cal/mol)	default
KMDegrdn	MicrobialDegrdn	rate of loss due to microbial degradation	(µg/L d)	site calib
KMDegrAnaerobic	KAnaerobic	decomposition rate at 0 g/m3 oxygen	(1/d)	site & calib
KUnCat	KUncat	the measured first-order reaction rate at pH 7	(1/d)	NA
KAcid	KAcidExp	pseudo-first-order acid-catalyzed rate constant for a given pH	(1/d)	NA
KBase	KBaseExp	pseudo-first-order rate constant for a given pH	(1/d)	NA
PhotolysisRate	KPhot	direct photolysis first-order rate constant	(1/d)	NA
OxRateConst	N / A	Not utilized as a parameter by the code.	(L/ mol d)	
KPSed	KPSed	detritus-water partition coefficient	(L/kg)	site & lit calc
Weibull_Shape	Shape	parameter expressing variability in toxic response	(unitless)	lit
ChemIsBase		if the compound is a base	(True/False)	NA
SiteRecord	**Site Underlying Data**	***For each Segment Simulated, the following parameters are required***		
SiteName	N / A	Site's Name. Used for Reference only.	N / A	
ECoeffWater	ExtinctH2O	light extinction of wavelength 312.5 nm in pure water	(1/m)	lit
SiteLength	Length	maximum effective length for wave setup, not used for Housatonic	(m)	
Volume	Volume	initial volume of site	(m^3)	EFDC
Area	Area	surface area of site (usually constant)	(m^2)	EFDC
ZMean	ZMean	mean depth	(m)	EFDC
ZMax	ZMax	maximum depth	(m)	EFDC
TempMean	TempMean	mean annual temperature	(°C)	site
TempRange	TempRange	annual temperature range	(°C)	site
Latitude	Latitude	latitude	(°, decimal)	site
LightMean	LightMean	mean annual light intensity	(ly/d)	site
LightRange	LightRange	annual range in light intensity	(ly/d)	site
AlkCaCO3	N / A	Not utilized as a parameter by the code.	mg/L	
HardCaCO3	N / A	Not utilized as a parameter by the code.	mg $CaCO_3$ / L	
SO4Conc	N / A	Not utilized as a parameter by the code.	mg/L	
TotalDissSolids	N / A	Not utilized as a parameter by the code.	mg/L	
StreamType	Stream Type	concrete channel, dredged channel, natural channel, not used for Housatonic	Choice from List	
Channel_Slope	Slope	slope of channel, not used for Housatonic	(m/m)	
Max_Chan_Depth	Max_Chan_Depth	depth at which flooding occurs , not used for Housatonic	(m)	
SedDepth	SedDepth	maximum sediment depth , not used for Housatonic	(m)	

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Internal to AQUATOX	Tech Doc Reference	Description	Units	Data Source
LimnoWallArea	LimnoWallArea	area of limnocorral walls; only relevant to limnocorral	(m^2)	NA
MeanEvap	MeanEvap	mean annual evaporation, not used for Housatonic	inches / year	
UseEnteredManning		do not determine Manning coefficient from streamtype, not used for Housatonic	(true/false)	
EnteredManning	Manning	manually entered Manning coefficient, not used for Housatonic	$s / m^{1/3}$	
ReminRecord	**Remineralization Data**	***For each simulation, the following parameters are required***		
DecayMax	DecayMax	maximum decomposition rate for detritus	(g/g·d)	lit
Q10	NA	Not utilized as a parameter by the code.	(unitless)	NA
TOpt	TOpt	optimum temperature	(°C)	lit
TMax	TMax	maximum temperature tolerated	(°C)	lit
TRef	NA	Not utilized as a parameter by the code.	(°C)	NA
pHMin	pHMin	minimum pH below which limitation on biodegradation rate occurs.	pH	lit
pHMax	pHMax	maximum pH above which limitation on biodegradation rate occurs.	pH	lit
Org2Phosphate	Org2Phosphate	ratio of phosphate to organic matter (unitless)	(unitless)	lit
Org2Ammonia	Org2Ammonia	ratio of ammonia to organic matter	(unitless)	lit
O2Biomass	O2Biomass	ratio of oxygen to organic matter	(unitless)	lit
O2N	O2N	ratio of oxygen to nitrogen	(unitless)	lit
KSed	KSed	intrinsic settling rate	(m/d)	EFDC
PSedRelease	N / A	Not utilized as a parameter by the code.	(g/m^2·d)	NA
NSedRelease	N / A	Not utilized as a parameter by the code.	(g/m^2·d)	NA
ZooRecord	**Animal Underlying Data**	***For each animal in the simulation, the following parameters are required***		
AnimalName	N / A	Animal's Name. Used for Reference only.	N / A	
FHalfSat	FHalfSat	half-saturation constant for feeding by a predator	(g/m^3)	calib
CMax	CMax	maximum feeding rate for predator	(g/g·d)	lit calc
BMin	BMin	minimum prey biomass needed to begin feeding	(g/m^3)	calib
Q10	Q10	slope or rate of change per 10°C temperature change	(unitless)	lit
TOpt	TOpt	optimum temperature	(°C)	lit
TMax	TMax	maximum temperature tolerated	(°C)	lit
TRef	TRef	adaptation temperature below which there is no acclimation	(°C)	lit
EndogResp	EndogResp	basal respiration rate at 0° C for given predator	(1/day)	lit calc
KResp	KResp	proportion assimilated energy lost to specific dynamic action	(unitless)	lit
KExcr	KExcr	proportionality constant for excretion:respiration	(unitless)	lit
PctGamete	PctGamete	fraction of adult predator biomass that is in gametes	(unitless)	lit & site
GMort	GMort	gamete mortality	(1/d)	site calib
KMort	KMort	intrinsic mortality rate	(g/g·d)	site calib
KCap	KCap	carrying capacity	(mg/L)	lit & site
MeanWeight	WetWt	mean wet weight of organism	(g)	site
FishFracLipid	LipidFrac	fraction of lipid in organism	(g lipid/g organism)	site & calc
LifeSpan	LifeSpan	mean lifespan in days	days	site
Animal_Type	Animal Type	Animal Type (Fish, Pelagic Invert, Benthic Invert, Benthic Insect)	Choice from List	
AveDrift	Dislodge	fraction of biomass subject to drift per day	fraction / day	lit
AutoSpawn		Should AQUATOX calculate Spawn Dates	(true/false)	prob. false

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Internal to AQUATOX	Tech Doc Reference	Description	Units	Data Source
SpawnDate1..3		Automatically Entered Spawn Dates	(date)	site
UnlimitedSpawning		Allow fish to spawn unlimited times each year	(true/false)	site
SpawnLimit		Number of spawns allowed for this species this year	(integer)	site
UseAllom_C		Use Allometric Consumption Equation	(true/false)	TRUE
CA		Allometric Consumption Parameter	(real number)	lit
CB		Allometric Consumption Parameter	(real number)	lit
UseAllom_R		Use Allometric Consumption Respiration	(true/false)	TRUE
RA		Allometric Respiration Parameter	(real number)	lit
RB		Allometric Respiration Parameter	(real number)	lit
UseSet1		Use "Set 1" of Allometric Respiration Parameters	(true/false)	lit
RQ		Allometric Respiration Parameter	(real number)	lit
RK1		Allometric Respiration Parameter	(real number)	lit
PlantRecord	**Plant Underlying Data**	***For each Plant in the Simulation, the following parameters are required***		
PlantName		Plant's Name. Used for Reference only.	N / A	
PlantType	Plant Type	Plant Type: (Phytoplankton, Periphyton, Macrophytes)	Choice from List	
LightSat	LightSat	light saturation level for photosynthesis	(ly/d)	lit & calib
KPO4	KP	half-saturation constant for phosphorus	(gP/m^3)	lit & calib
KN	KN	half-saturation constant for nitrogen	(gN/m^3)	lit & calib
KCarbon	KCO2	half-saturation constant for carbon	(gC/m^3)	lit & calib
Q10	Q10	slope or rate of change per 10°C temperature change	(unitless)	lit
TOpt	TOpt	optimum temperature	(°C)	lit
TMax	TMax	maximum temperature tolerated	(°C)	lit
TRef	TRef	adaptation temperature below which there is no acclimation	(°C)	lit
PMax	PMax	maximum photosynthetic rate	(1/d)	lit
KResp	KResp	coefficient of proportionality btwn. excretion and photosynthesis at optimal light levels	(unitless)	lit
KMort	KMort	intrinsic mortality rate	(g/g·d)	calib
EMort	EMort	exponential factor for suboptimal conditions	(unitless)	calib
KSed	KSed	intrinsic settling rate	(m/d)	lit
ESed	ESed	exponential settling coefficient	(unitless)	lit
UptakePO4	Uptake $_{Phosphorus}$	fraction of photosynthate that is nutrient	(unitless)	lit
UptakeN	Uptake $_{Nitrogen}$	fraction of photosynthate that is nutrient	(unitless)	lit
ECoeffPhyto	EcoeffPhyto	attenuation coefficient for given alga	($1/m\text{-}g/m^3$)	lit
CarryCapac	KCap	carrying capacity of periphyton	(g/m^2)	site
Red_Still_Water	RedStillWater	reduction in photosynthesis in absence of current	(unitless)	lit
Macrophyte_Type	Macrophyte Type	Type of macrophyte (benthic, rooted floating, free-floating)	Choice from List	site
TAnimalToxRecord	**Animal Toxicity Parameters**	***For each Chemical Simulated, the following parameters are required for each animal in the model***		
LC50	LC50	external concentration of toxicant at which 50% of population is killed *	(µg/L)	site & lit
LC50_exp_time	ObsTElapsed	exposure time in toxicity determination *	(h)	site & lit
K2	K2	elimination rate constant	(1/d)	calc & calib
Bio_rate_const : Double;	Biotransformation Rate		(1/d)	lit & calib
EC50_growth	EC50Growth	external concentration of toxicant at which there is a 50% reduction in growth *	(µg/L)	site & lit

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Internal to AQUATOX	Tech Doc Reference	Description	Units	Data Source
Growth_exp_time	ObsTElapsed	exposure time in toxicity determination *	(h)	site & lit
EC50_repro	EC50Repro	external concentration of toxicant at which there is a 50% reduction in reproduction *	(µg/L)	site & lit
Repro_exp_time	ObsTElapsed	exposure time in toxicity determination *	(h)	site & lit
Ave_wet_wt	WetWt	mean wet weight of organism	(g)	site
Lipid_frac	LipidFrac	fraction of lipid in organism	(g lipid/g organism)	site & calc
Drift_Thresh	Drift Threshold	concentration at which drift is initiated *	(µg/L)	lit & calib
		*** prob. not used for Housatonic**		
TPlantToxRecord	**Plant Toxicity Parameters**	***For each Chemical Simulated, the following parameters are required for each plant in the model***		
EC50_photo	EC50Photo	external concentration of toxicant at which there is 50% reduction in photosynthesis *	(µg/L)	lit
EC50_exp_time	ObsTElapsed	exposure time in toxicity determination *	(h)	lit
K2	K2	elimination rate constant	(1/d)	lit & calib
Bio_rate_const	Biotransformation Rate		(1/d)	lit & calib
LC50	LC50	external concentration of toxicant at which 50% of population is killed *	(µg/L)	lit & site
LC50_exp_time	ObsTElapsed	exposure time in toxicity determination *	(h)	lit & site
Lipid_frac	LipidFrac	fraction of lipid in organism	(g lipid/g organism)	lit & site
		*** prob. not used for Housatonic**		
TBioTransRecord	**Biotransformation Params.**	***For each type of Biotransformation to be simulated, the following parameters are required***		
BTType	Category of Biotransformation	AerobicMicrobial, AnaerobicMicrobial, Algae, BenthInsect, OtherBenthos, Fish, UserSpecifi	Choice from List	lit & calib
UserSpec	User Specified Species	If this type of biotransf. occurs in user specified species, that species chosen here	Choice from List	lit & calib
Percent	Biotransformation to	Of total biotransformation within this category, the % transformed to various chemicals	Set of Percentages	lit & calib
TChemical	**Chemical**	***For each Chemical to be simulated, the following are required***		
InitialCond	Initial Condition	Initial Condition of the state variable	µg/L	site
Loadings	Inflow Loadings	Daily loading as a result of the inflow of water (excluding modeled upstream reaches)	µg/L	HSPF
Alt_Loadings[Pointsource]	Point Source Loadings	Daily loading from point sources	(g/d)	HSPF
Alt_Loadings[Direct Precip]	Direct Precipitation Loadings	Daily loading from direct precipitation	($g/m^2 \cdot d$)	site
Alt_Loadings[NonPointsource]	Non-Point Source Loadings	Daily loading from non-point sources	(g/d)	HSPF
Tox_Air	Gas-phase concentration	will prob. ignore for Housatonic	(g/m^3)	site & lit
TRemineralize	**Nutrient**	***For each Nutrient to be simulated, including O_2 and CO_2, the following are required***		
InitialCond	Initial Condition	Initial Condition of the state variable	mg/L	site
Loadings	Inflow Loadings	Daily loading as a result of the inflow of water (excluding modeled upstream reaches)	mg/L	HSPF
Alt_Loadings[Pointsource]	Point Source Loadings	Daily loading from point sources	(g/d)	HSPF
Alt_Loadings[Direct Precip]	Direct Precipitation Loadings	Daily loading from direct precipitation; will prob. ignore for Housatonic	($g/m^2 \cdot d$)	site
Alt_Loadings[NonPointsource]	Non-Point Source Loadings	Daily loading from non-point sources	(g/d)	HSPF
TSedDetr	**Sed. Detritus Parameters**	***For Sedimented POM the following parameters are required***		
InitialCond	Initial Condition	Initial Condition of the state variable	(g/m^2)	site
TToxicant.InitialCond	Toxicant Exposure	Initial Toxicant Exposure of the state variable, for each chemical simulated	µg/kg	site
TDetritus	**Susp & Dissolved Detritus**	***For the Suspended and Dissolved Detritus compartments, the following parameters are required***		
InitialCond	Initial Condition	Initial Cond. of susp. & diss. detritus, as organic matter, organic carbon, or BOD	mg/L	site

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AQUATOX Parameter List

Internal to AQUATOX	Tech Doc Reference	Description	Units	Data Source
Percent_Part_IC	Percent Particulate $_{\text{Init Cond}}$	Percent of Initial Condition that is particulate as opposed to dissolved detritus	percentage	site
Loadings	Inflow Loadings	Daily loading as a result of the inflow of water (excluding modeled upstream reaches)	mg/L	HSPF
Percent_Part	Percent Particulate $_{\text{Inflow}}$	Daily parameter; % of loading that is particulate as opposed to dissolved detritus	percentage	site
Alt_Loadings[Pointsource]	Point Source Loadings	Daily loading from point sources	(g/d)	HSPF
Percent_Part_PS	Percent Particulate $_{\text{PointSrc}}$	Daily parameter; % of loading that is particulate as opposed to dissolved detritus	percentage	site
Alt_Loadings[NonPointsource]	Non-Point Source Loadings	Daily loading from non-point sources	(g/d)	HSPF
Percent_Part_NPS	Percent Particulate $_{\text{NonPointSrc}}$	Daily parameter; % of loading that is particulate as opposed to dissolved detritus	percentage	site
TToxicant.InitialCond	Toxicant Exposure	Initial Toxicant concentration of the state variable	µg/kg	site
TToxicant.Loads	Tox Exposure of Inflow Load	Daily parameter; Tox. concentration of each type of inflowing detritus, for each chemical	µg/kg	site
TBuried Detritus	**Buried Detritus**	***For Each Layer of Buried Detritus, the following parameters are required***		
InitialCond	Initial Condition	Initial Condition of the state variable	(g/m^2)	site
TToxicant.InitialCond	Toxicant Exposure	Initial Toxicant concentration of the state variable, for each chemical simulated	µg/kg	site
TPlant	**Plant Parameters**	***For each plant type simulated, the following parameters are required***		
InitialCond	Initial Condition	Initial Condition of the state variable	mg/L	site
Loadings	Inflow Loadings	Daily loading as a result of the inflow of water (excluding modeled upstream reaches)	mg/L	site
TToxicant.InitialCond	Toxicant Exposure	Initial Toxicant concentration of the state variable	µg/kg	site
TToxicant.Loads	Tox Exposure of Inflow Load	Daily parameter; Tox. concentration of the Inflow Loadings, for each chemical	µg/kg	site
TAnimal	**Animal Parameters**	***For each animal type simulated, the following parameters are required***		
InitialCond	Initial Condition	Initial Condition of the state variable	mg/L	site
Loadings	Inflow Loadings	Daily loading as a result of the inflow of water (excluding modeled upstream reaches)	mg/L	site
TToxicant.InitialCond	Toxicant Exposure	Initial Toxicant concentration of the state variable	µg/kg	site
TToxicant.Loads	Tox Exposure of Inflow Load	Daily parameter; Tox. concentration of the Inflow Loadings, for each chemical simulated	µg/kg	site
TrophIntArray.Pref	$\text{Pref}_{\text{prey, pred}}$	for each prey-type ingested, a preference value within the matrix of preference parameters	(unitless)	lit
TrophIntArray.ECoeff	EgestCoeff	for each prey-type ingested, the fraction of ingested prey that is egested	(unitless)	lit
TVolume	**Volume Parameters**	***For each segment simulated, the following water flow parameters are required***		
InitialCond	Initial Condition	Initial Condition of the state variable	(m^3)	site
InflowLoad	Inflow of Water	Inflow of water, excluding upstream linked segments	(m^3/d)	EFDC
DischargeLoad	Discharge of Water	Discharge of water, excluding downstream linked segments	(m^3/d)	EFDC
FlowToFlood	FlowToFlood	Daily parameter; water flow into the floodplain during flood events	(m^3/d)	EFDC
FlowFromFlood	FlowFromFlood	Daily parameter; water flow out of the floodplain during flood events	(m^3/d)	EFDC
Site Characteristics	**Site Characteristics**	***For each segment simulated, the following characteristics parameters are required***		
Temperature	Temperature	Daily parameter; temperature of the segment; ***Optional***, can use annual mean	(°C)	site
Wind	Wind	Daily parameter; wind velocity 10 m above the water; ***Optional***, default time series avail.	(m/s)	site
Light	Light	Daily parameter; avg. light intensity at segment top; ***Optional***, can use annual Mean and Range	(ly/d)	site
Photoperiod	Photoperiod	Fraction of day with daylight; ***Optional***, can be calculated from latitude	(hr/d)	calc.
pH	pH	Daily parameter; pH of the segment.	(pH)	site

Appendix D.2

AQUATOX Parameter List

Internal to AQUATOX	Tech Doc Reference	Description	Units	Data Source
Physical Geometry	**Physical Geometry**	***For each segment simulated, the following physical geometry parameters are required for each day***		
Thickness	Segment Thickness	Thickness of the segment	m	EFDC
XSection	Cross Section Area	Cross sectional area of the segment	(m^2)	EFDC
Surface Area	Surface Area	Surface area of the segment	(m^2)	EFDC
TSegmentLink	**Segment Link Parameters**	***For each Link between two Segments, the following parameters are required***		
LinkType	Link Type	Is this a "Cascade Link" or a "Feedback Link"	Choice from List	site
FromID, ToID	Link Location	Describes which segments are linked together	Choice from List	site
Length	Length	Characteristic Length	(m)	site
XSectionData	Cross Section Loadings	Cross Sectional Area for each day of simulation	(m^2)	EFDC
DiffusionData	Diffusion Loadings	Daily Dispersion Coefficient	(m^2/d)	EFDC
WaterFlowData	Water Flow Loadings	Daily water flow through the linkage	(m^3/d)	EFDC
TSedimentData	**Sediment Data Parameters**	***For each AQUATOX segment, for each sediment modeled, the following parameters are required each day***		
Loading	External Loading	external load of this suspended sediment type (not from upstream link)	(g/d)	HSPF
BedLoad	BedLoad	bed load of cohesive and noncohesive sediments	(g/d)	EFDC
Deposition	Deposition	net deposition of cohesive and noncohesive sediments	(g/d)	EFDC
Resuspension	Resuspension	net resuspension of cohesive and noncohesive sediments	(g/d)	EFDC
LErodVel	Erosion Velocity	erosional velocity for cohesive sediments	(m/d)	EFDC
LDepVel	Deposition Velocity	depositional velocity for cohesive sediments	(m/d)	EFDC
TStates (sed. parmameters)	**Sediment Model Parameters**	***For each AQUATOX segment, the following parameters are required***		
MaxUpperThick	MaxThick	maximum thickness of the active layer	(m)	site & lit
BioturbThick	Bioturbation Depth	depth at which bioturbation takes place, also the minimum thickness for this layer	(m)	site & lit
TBuriedSedimentData	**Sediment Layer Parameters**	***For each Sediment Layer modeled in each segment, the following parameters are required***		
BedDepthIC	Thickness	initial condition thickness of the sediment layer	(m)	site
CharLength	Characteristic Length	characteristic length of the interface with above water or above sediment layer	(m)	site
UpperDispCoeff	Dispersion Coefficient	dispersion coefficient for interface with above water or above sediment layer	(m^2/d)	site & lit
InitCond	Initial Conditions	initial conditions for each type of sediment modeled (organic and inorganic)	(g/m^2)	site
Tox InitCond	Toxicant Init. Conditions	initial conditions for toxicant concentration in each type of sediment modeled	µg/kg	site
TPoreWater	**Pore Water Parameters**	***For each Sediment Layer modeled in each segment, the following pore water parameters are required***		
PoreWaterIC	Initial condition	initial quantity of pore water in the sediment layer	(m^2 / m^3)	site
TDOMPoreWater	DOM Init. Condition	initial quantity of DOM in the pore water	(g / m^3)	site
Tox InitCond	Toxicant Init. Conditions	initial conditions for toxicant concentration in above pore water compartments	µg/kg	site
TSediment	**Density Parameters**	***For each type of sediment modeled, (organic and inorganic)***		
Densities[ ]	Density	the density of this sediment within the sediment bed	g/m3	site & lit